

Package ‘mlr3tuning’

June 26, 2023

Title Hyperparameter Optimization for 'mlr3'

Version 0.19.0

Description Hyperparameter optimization package of the 'mlr3' ecosystem. It features highly configurable search spaces via the 'paradox' package and finds optimal hyperparameter configurations for any 'mlr3' learner. 'mlr3tuning' works with several optimization algorithms e.g. Random Search, Iterated Racing, Bayesian Optimization (in 'mlr3mbo') and Hyperband (in 'mlr3hyperband'). Moreover, it can automatically optimize learners and estimate the performance of optimized models with nested resampling.

License LGPL-3

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

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

Depends mlr3 (>= 0.14.1), paradox (>= 0.10.0), R (>= 3.1.0)

Imports bbotk (>= 0.7.2), checkmate (>= 2.0.0), data.table, lgr,
mlr3misc (>= 0.11.0), R6

Suggests adagio, GenSA, irace, knitr, mlr3learners (>= 0.5.5),
mlr3pipelines, nloptr, rmarkdown, rpart, testthat (>= 3.0.0),
xgboost

Config/testthat/edition 3

Config/testthat/parallel true

Encoding UTF-8

NeedsCompilation no

RoxygenNote 7.2.3

Collate 'ArchiveTuning.R' 'AutoTuner.R' 'CallbackTuning.R'
'ContextEval.R' 'ObjectiveTuning.R' 'mlr_tuners.R' 'Tuner.R'
'TunerCmaes.R' 'TunerDesignPoints.R' 'TunerFromOptimizer.R'
'TunerGenSA.R' 'TunerGridSearch.R' 'TunerIrace.R'
'TunerNLOptr.R' 'TunerRandomSearch.R'
'TuningInstanceSingleCrit.R' 'TuningInstanceMulticrit.R'

'as_search_space.R' 'assertions.R' 'auto_tuner.R'
 'bibentries.R' 'extract_inner_tuning_archives.R'
 'extract_inner_tuning_results.R' 'helper.R' 'mlr_callbacks.R'
 'reexport.R' 'sugar.R' 'tune.R' 'tune_nested.R' 'zzz.R'

VignetteBuilder knitr

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 2023-06-26 16:50:02 UTC

R topics documented:

mlr3tuning-package	3
ArchiveTuning	3
as_search_space	7
AutoTuner	7
auto_tuner	13
CallbackTuning	16
callback_tuning	17
ContextEval	19
extract_inner_tuning_archives	21
extract_inner_tuning_results	22
mlr3tuning.backup	24
mlr3tuning.early_stopping	25
mlr3tuning.measures	26
mlr_tuners	27
mlr_tuners_cmaes	28
mlr_tuners_design_points	30
mlr_tuners_gensa	32
mlr_tuners_grid_search	35
mlr_tuners_irace	37
mlr_tuners_nloptr	40
mlr_tuners_random_search	43
ObjectiveTuning	45
ti	47
tnr	50
tune	51
Tuner	54
tune_nested	58
TuningInstanceMultiCrit	60
TuningInstanceSingleCrit	63

Index

68

mlr3tuning-package *mlr3tuning: Hyperparameter Optimization for 'mlr3'*

Description

Hyperparameter optimization package of the 'mlr3' ecosystem. It features highly configurable search spaces via the 'paradox' package and finds optimal hyperparameter configurations for any 'mlr3' learner. 'mlr3tuning' works with several optimization algorithms e.g. Random Search, Iterated Racing, Bayesian Optimization (in 'mlr3mbo') and Hyperband (in 'mlr3hyperband'). Moreover, it can automatically optimize learners and estimate the performance of optimized models with nested resampling.

Author(s)

Maintainer: Marc Becker <marcbecker@posteo.de> ([ORCID](#))

Authors:

- Michel Lang <michellang@gmail.com> ([ORCID](#))
- Jakob Richter <jakob1richter@gmail.com> ([ORCID](#))
- Bernd Bischl <bernd_bischl@gmx.net> ([ORCID](#))
- Daniel Schalk <daniel.schalk@stat.uni-muenchen.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>

ArchiveTuning

Class for Logging Evaluated Hyperparameter Configurations

Description

The [ArchiveTuning](#) stores all evaluated hyperparameter configurations and performance scores.

Details

The [ArchiveTuning](#) is a container around a `data.table::data.table()`. Each row corresponds to a single evaluation of a hyperparameter configuration. See the section on Data Structure for more information. The archive stores additionally a `mlr3::BenchmarkResult` (`$benchmark_result`) that records the resampling experiments. Each experiment corresponds to a single evaluation of a hyperparameter configuration. The table (`$data`) and the benchmark result (`$benchmark_result`) are linked by the `uhash` column. If the archive is passed to `as.data.table()`, both are joined automatically.

Data Structure

The table (`$data`) has the following columns:

- One column for each hyperparameter of the search space (`$search_space`).
- One column for each performance measure (`$codomain`).
- `x_domain(list())`
Lists of (transformed) hyperparameter values that are passed to the learner.
- `runtime_learners(numeric(1))`
Sum of training and predict times logged in learners per `mlr3::ResampleResult` / evaluation. This does not include potential overhead time.
- `timestamp(POSIXct)`
Time stamp when the evaluation was logged into the archive.
- `batch_nr(integer(1))`
Hyperparameters are evaluated in batches. Each batch has a unique batch number.
- `uhash(character(1))`
Connects each hyperparameter configuration to the resampling experiment stored in the `mlr3::BenchmarkResult`.

Analysis

For analyzing the tuning results, it is recommended to pass the `ArchiveTuning` to `as.data.table()`. The returned data table is joined with the benchmark result which adds the `mlr3::ResampleResult` for each hyperparameter evaluation.

The archive provides various getters (e.g. `$learners()`) to ease the access. All getters extract by position (`i`) or unique hash (`uhash`). For a complete list of all getters see the methods section.

The benchmark result (`$benchmark_result`) allows to score the hyperparameter configurations again on a different measure. Alternatively, measures can be supplied to `as.data.table()`.

The `mlr3viz` package provides visualizations for tuning results.

S3 Methods

- `as.data.table.ArchiveTuning(x, unnest = "x_domain", exclude_columns = "uhash", measures = NULL)`
Returns a tabular view of all evaluated hyperparameter configurations.
`ArchiveTuning -> data.table::data.table()`
 - `x(ArchiveTuning)`
 - `unnest(character())`
Transforms list columns to separate columns. Set to `NULL` if no column should be unnested.
 - `exclude_columns(character())`
Exclude columns from table. Set to `NULL` if no column should be excluded.
 - `measures(List of mlr3::Measure)`
Score hyperparameter configurations on additional measures.

Super class

`bbotk::Archive -> ArchiveTuning`

Public fields

benchmark_result ([mlr3::BenchmarkResult](#))
Benchmark result.

Methods**Public methods:**

- [ArchiveTuning\\$new\(\)](#)
- [ArchiveTuning\\$learner\(\)](#)
- [ArchiveTuning\\$learners\(\)](#)
- [ArchiveTuning\\$learner_param_vals\(\)](#)
- [ArchiveTuning\\$predictions\(\)](#)
- [ArchiveTuning\\$resample_result\(\)](#)
- [ArchiveTuning\\$print\(\)](#)
- [ArchiveTuning\\$clone\(\)](#)

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

Usage:

```
ArchiveTuning$new(search_space, codomain, check_values = TRUE)
```

Arguments:

search_space ([paradox::ParamSet](#))

Hyperparameter search space. If NULL (default), the search space is constructed from the [TuneToken](#) of the learner's parameter set (`learner$param_set`).

codomain ([bbotk::Codomain](#))

Specifies codomain of objective function i.e. a set of performance measures. Internally created from provided [mlr3::Measures](#).

check_values (`logical(1)`)

If TRUE (default), hyperparameter configurations are check for validity.

Method `learner()`: Retrieve [mlr3::Learner](#) of the i-th evaluation, by position or by unique hash uhash. i and uhash are mutually exclusive. Learner does not contain a model. Use `$learners()` to get learners with models.

Usage:

```
ArchiveTuning$learner(i = NULL, uhash = NULL)
```

Arguments:

i (`integer(1)`)

The iteration value to filter for.

uhash (`logical(1)`)

The uhash value to filter for.

Method `learners()`: Retrieve list of trained [mlr3::Learner](#) objects of the i-th evaluation, by position or by unique hash uhash. i and uhash are mutually exclusive.

Usage:

```
ArchiveTuning$learners(i = NULL, uhash = NULL)
```

Arguments:

`i` (integer(1))
The iteration value to filter for.

`uhash` (logical(1))
The uhash value to filter for.

Method `learner_param_vals()`: Retrieve param values of the `i`-th evaluation, by position or by unique hash `uhash`. `i` and `uhash` are mutually exclusive.

Usage:

```
ArchiveTuning$learner_param_vals(i = NULL, uhash = NULL)
```

Arguments:

`i` (integer(1))
The iteration value to filter for.

`uhash` (logical(1))
The uhash value to filter for.

Method `predictions()`: Retrieve list of [mlr3::Prediction](#) objects of the `i`-th evaluation, by position or by unique hash `uhash`. `i` and `uhash` are mutually exclusive.

Usage:

```
ArchiveTuning$predictions(i = NULL, uhash = NULL)
```

Arguments:

`i` (integer(1))
The iteration value to filter for.

`uhash` (logical(1))
The uhash value to filter for.

Method `resample_result()`: Retrieve [mlr3::ResampleResult](#) of the `i`-th evaluation, by position or by unique hash `uhash`. `i` and `uhash` are mutually exclusive.

Usage:

```
ArchiveTuning$resample_result(i = NULL, uhash = NULL)
```

Arguments:

`i` (integer(1))
The iteration value to filter for.

`uhash` (logical(1))
The uhash value to filter for.

Method `print()`: Printer.

Usage:

```
ArchiveTuning$print()
```

Arguments:

... (ignored).

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

as_search_space	<i>Convert to a Search Space</i>
-----------------	----------------------------------

Description

Convert object to a search space.

Usage

```
as_search_space(x, ...)
```

```
## S3 method for class 'Learner'
```

```
as_search_space(x, ...)
```

```
## S3 method for class 'ParamSet'
```

```
as_search_space(x, ...)
```

Arguments

x	(any) Object to convert to search space.
...	(any) Additional arguments.

Value

[paradox::ParamSet](#).

AutoTuner	<i>Class for Automatic Tuning</i>
-----------	-----------------------------------

Description

The [AutoTuner](#) wraps a [mlr3::Learner](#) and augments it with an automatic tuning process for a given set of hyperparameters. The `auto_tuner()` function creates an [AutoTuner](#) object.

Details

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 stored in `at$learner`. Access the tuned hyperparameters via `at$tuning_result`.

3. A final model is fit on the complete training data using the now parametrized wrapped learner. The respective model is available via field at `$learner$model`.

During `$predict()` the `AutoTuner` just calls the `predict` method of the wrapped (inner) learner. A set timeout is disabled while fitting the final model.

Resources

There are several sections about hyperparameter optimization in the [mlr3book](#).

- [Automate](#) the tuning.
- Estimate the model performance with [nested resampling](#).

The [gallery](#) features a collection of case studies and demos about optimization.

Nested Resampling

Nested resampling is performed by passing an `AutoTuner` 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). The `mlr3::Resampling` passed to the `AutoTuner` is meant to be the inner resampling, operating on the training set of an arbitrary outer resampling. For this reason, the inner resampling should be not instantiated. If an instantiated resampling is passed, the `AutoTuner` fails when a row id of the inner resampling is not present in the training set of the outer resampling.

Default Measures

If no measure is passed, the default measure is used. The default measure depends on the task type.

Task	Default Measure	Package
"classif"	"classif.ce"	mlr3
"regr"	"regr.mse"	mlr3
"surv"	"surv.cindex"	mlr3proba
"dens"	"dens.logloss"	mlr3proba
"classif_st"	"classif.ce"	mlr3spatial
"regr_st"	"regr.mse"	mlr3spatial
"clust"	"clust.dunn"	mlr3cluster

Super class

`mlr3::Learner` -> `AutoTuner`

Public fields

`instance_args` (`list()`)

All arguments from construction to create the `TuningInstanceSingleCrit`.

`tuner` (`Tuner`)

Optimization algorithm.

Active bindings

- archive ([ArchiveTuning](#))
Archive of the [TuningInstanceSingleCrit](#).
- learner ([mlr3::Learner](#))
Trained learner
- tuning_instance ([TuningInstanceSingleCrit](#))
Internally created tuning instance with all intermediate results.
- tuning_result ([data.table::data.table](#))
Short-cut to result from [TuningInstanceSingleCrit](#).
- predict_type (character(1))
Stores the currently active predict type, e.g. "response". Must be an element of `$predict_types`.
- hash (character(1))
Hash (unique identifier) for this object.
- phash (character(1))
Hash (unique identifier) for this partial object, excluding some components which are varied systematically during tuning (parameter values) or feature selection (feature names).

Methods**Public methods:**

- [AutoTuner\\$new\(\)](#)
- [AutoTuner\\$base_learner\(\)](#)
- [AutoTuner\\$importance\(\)](#)
- [AutoTuner\\$selected_features\(\)](#)
- [AutoTuner\\$soob_error\(\)](#)
- [AutoTuner\\$loglik\(\)](#)
- [AutoTuner\\$print\(\)](#)
- [AutoTuner\\$clone\(\)](#)

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

Usage:

```
AutoTuner$new(
  tuner,
  learner,
  resampling,
  measure = NULL,
  terminator,
  search_space = NULL,
  store_tuning_instance = TRUE,
  store_benchmark_result = TRUE,
  store_models = FALSE,
  check_values = FALSE,
  allow_hotstart = FALSE,
  keep_hotstart_stack = FALSE,
  evaluate_default = FALSE,
```

```

    callbacks = list()
  )

```

Arguments:

tuner ([Tuner](#))
Optimization algorithm.

learner ([mlr3::Learner](#))
Learner to tune.

resampling ([mlr3::Resampling](#))
Resampling that is used to evaluate the performance of the hyperparameter configurations. Uninstantiated resamplings are instantiated during construction so that all configurations are evaluated on the same data splits. Already instantiated resamplings are kept unchanged. Specialized [Tuner](#) change the resampling e.g. to evaluate a hyperparameter configuration on different data splits. This field, however, always returns the resampling passed in construction.

measure ([mlr3::Measure](#))
Measure to optimize. If NULL, default measure is used.

terminator ([Terminator](#))
Stop criterion of the tuning process.

search_space ([paradox::ParamSet](#))
Hyperparameter search space. If NULL (default), the search space is constructed from the [TuneToken](#) of the learner's parameter set (learner\$param_set).

store_tuning_instance (logical(1))
If TRUE (default), stores the internally created [TuningInstanceSingleCrit](#) with all intermediate results in slot \$tuning_instance.

store_benchmark_result (logical(1))
If TRUE (default), store resample result of evaluated hyperparameter configurations in archive as [mlr3::BenchmarkResult](#).

store_models (logical(1))
If TRUE, fitted models are stored in the benchmark result (archive\$benchmark_result). If store_benchmark_result = FALSE, models are only stored temporarily and not accessible after the tuning. This combination is needed for measures that require a model.

check_values (logical(1))
If TRUE, hyperparameter values are checked before evaluation and performance scores after. If FALSE (default), values are unchecked but computational overhead is reduced.

allow_hotstart (logical(1))
Allow to hotstart learners with previously fitted models. See also [mlr3::HotstartStack](#). The learner must support hotstarting. Sets store_models = TRUE.

keep_hotstart_stack (logical(1))
If TRUE, [mlr3::HotstartStack](#) is kept in \$objective\$hotstart_stack after tuning.

evaluate_default (logical(1))
If TRUE, learner is evaluated with hyperparameters set to their default values at the start of the optimization.

callbacks (list of [CallbackTuning](#))
List of callbacks.

Method `base_learner()`: Extracts the base learner from nested learner objects like `GraphLearner` in [mlr3pipelines](#). If `recursive = 0`, the (tuned) learner is returned.

Usage:

```
AutoTuner$base_learner(recursive = Inf)
```

Arguments:

```
recursive (integer(1))  
  Depth of recursion for multiple nested objects.
```

Returns: [Learner](#).

Method `importance()`: The importance scores of the final model.

Usage:

```
AutoTuner$importance()
```

Returns: Named numeric().

Method `selected_features()`: The selected features of the final model.

Usage:

```
AutoTuner$selected_features()
```

Returns: character().

Method `oob_error()`: The out-of-bag error of the final model.

Usage:

```
AutoTuner$oob_error()
```

Returns: numeric(1).

Method `loglik()`: The log-likelihood of the final model.

Usage:

```
AutoTuner$loglik()
```

Returns: logLik. Printer.

Method `print()`:

Usage:

```
AutoTuner$print()
```

Arguments:

```
... (ignored).
```

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

```
# Automatic Tuning

# split to train and external set
task = tsk("penguins")
split = partition(task, ratio = 0.8)

# load learner and set search space
learner = lrn("classif.rpart",
  cp = to_tune(1e-04, 1e-1, logscale = TRUE)
)

# create auto tuner
at = auto_tuner(
  tuner = tnr("random_search"),
  learner = learner,
  resampling = rsmp("holdout"),
  measure = msr("classif.ce"),
  term_evals = 4)

# tune hyperparameters and fit final model
at$train(task, row_ids = split$train)

# predict with final model
at$predict(task, row_ids = split$test)

# show tuning result
at$tuning_result

# model slot contains trained learner and tuning instance
at$model

# shortcut trained learner
at$learner

# shortcut tuning instance
at$tuning_instance

# Nested Resampling

at = auto_tuner(
  tuner = tnr("random_search"),
  learner = learner,
  resampling = rsmp("holdout"),
  measure = msr("classif.ce"),
  term_evals = 4)

resampling_outer = rsmp("cv", folds = 3)
rr = resample(task, at, resampling_outer, store_models = TRUE)

# retrieve inner tuning results.
```

```
extract_inner_tuning_results(rr)

# performance scores estimated on the outer resampling
rr$score()

# unbiased performance of the final model trained on the full data set
rr$aggregate()
```

auto_tuner

Function for Automatic Tuning

Description

The [AutoTuner](#) wraps a [mlr3::Learner](#) and augments it with an automatic tuning process for a given set of hyperparameters. The `auto_tuner()` function creates an [AutoTuner](#) object.

Usage

```
auto_tuner(
  tuner,
  learner,
  resampling,
  measure = NULL,
  term_evals = NULL,
  term_time = NULL,
  terminator = NULL,
  search_space = NULL,
  store_tuning_instance = TRUE,
  store_benchmark_result = TRUE,
  store_models = FALSE,
  check_values = FALSE,
  allow_hotstart = FALSE,
  keep_hotstart_stack = FALSE,
  evaluate_default = FALSE,
  callbacks = list(),
  method
)
```

Arguments

tuner	(Tuner) Optimization algorithm.
learner	(mlr3::Learner) Learner to tune.
resampling	(mlr3::Resampling) Resampling that is used to evaluate the performance of the hyperparameter configurations. Uninstantiated resamplings are instantiated during construction so

that all configurations are evaluated on the same data splits. Already instantiated resamplings are kept unchanged. Specialized [Tuner](#) change the resampling e.g. to evaluate a hyperparameter configuration on different data splits. This field, however, always returns the resampling passed in construction.

measure	(mlr3::Measure) Measure to optimize. If NULL, default measure is used.
term_evals	(integer(1)) Number of allowed evaluations. Ignored if terminator is passed.
term_time	(integer(1)) Maximum allowed time in seconds. Ignored if terminator is passed.
terminator	(Terminator) Stop criterion of the tuning process.
search_space	(paradox::ParamSet) Hyperparameter search space. If NULL (default), the search space is constructed from the TuneToken of the learner's parameter set (learner\$param_set).
store_tuning_instance	(logical(1)) If TRUE (default), stores the internally created TuningInstanceSingleCrit with all intermediate results in slot \$tuning_instance.
store_benchmark_result	(logical(1)) If TRUE (default), store resample result of evaluated hyperparameter configurations in archive as mlr3::BenchmarkResult .
store_models	(logical(1)) If TRUE, fitted models are stored in the benchmark result (archive\$benchmark_result). If store_benchmark_result = FALSE, models are only stored temporarily and not accessible after the tuning. This combination is needed for measures that require a model.
check_values	(logical(1)) If TRUE, hyperparameter values are checked before evaluation and performance scores after. If FALSE (default), values are unchecked but computational overhead is reduced.
allow_hotstart	(logical(1)) Allow to hotstart learners with previously fitted models. See also mlr3::HotstartStack . The learner must support hotstarting. Sets store_models = TRUE.
keep_hotstart_stack	(logical(1)) If TRUE, mlr3::HotstartStack is kept in \$objective\$hotstart_stack after tuning.
evaluate_default	(logical(1)) If TRUE, learner is evaluated with hyperparameters set to their default values at the start of the optimization.
callbacks	(list of CallbackTuning) List of callbacks.

method (character(1))
 Deprecated. Use tuner instead.

Details

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 stored in `at$learner`. Access the tuned hyperparameters via `at$tuning_result`.
3. A final model is fit on the complete training data using the now parametrized wrapped learner. The respective model is available via field `at$learner$model`.

During `$predict()` the `AutoTuner` just calls the `predict` method of the wrapped (inner) learner. A set timeout is disabled while fitting the final model.

Value

`AutoTuner`.

Default Measures

If no measure is passed, the default measure is used. The default measure depends on the task type.

Task	Default Measure	Package
"classif"	"classif.ce"	mlr3
"regr"	"regr.mse"	mlr3
"surv"	"surv.cindex"	mlr3proba
"dens"	"dens.logloss"	mlr3proba
"classif_st"	"classif.ce"	mlr3spatial
"regr_st"	"regr.mse"	mlr3spatial
"clust"	"clust.dunn"	mlr3cluster

Resources

There are several sections about hyperparameter optimization in the [mlr3book](#).

- [Automate](#) the tuning.
- Estimate the model performance with [nested resampling](#).

The [gallery](#) features a collection of case studies and demos about optimization.

Nested Resampling

Nested resampling is performed by passing an `AutoTuner` 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). The `mlr3::Resampling` passed to the `AutoTuner` is meant to be the inner resampling, operating on the training set of an arbitrary outer resampling. For this reason, the inner resampling should be not instantiated. If an instantiated resampling is passed, the `AutoTuner` fails when a row id of the inner resampling is not present in the training set of the outer resampling.

Examples

```
at = auto_tuner(
  tuner = tnr("random_search"),
  learner = lrn("classif.rpart", cp = to_tune(1e-04, 1e-1, logscale = TRUE)),
  resampling = rsmp("holdout"),
  measure = msr("classif.ce"),
  term_evals = 4)

at$train(tsk("pima"))
```

CallbackTuning

Create Tuning Callback

Description

Specialized `bbotk::CallbackOptimization` for tuning. Callbacks allow to customize the behavior of processes in `mlr3tuning`. The `callback_tuning()` function creates a `CallbackTuning`. Predefined callbacks are stored in the dictionary `mlr_callbacks` and can be retrieved with `clbk()`. For more information on tuning callbacks see `callback_tuning()`.

Super classes

`mlr3misc::Callback` -> `bbotk::CallbackOptimization` -> `CallbackTuning`

Public fields

`on_eval_after_design` (function())

Stage called after design is created. Called in `ObjectiveTuning$eval_many()`.

`on_eval_after_benchmark` (function())

Stage called after hyperparameter configurations are evaluated. Called in `ObjectiveTuning$eval_many()`.

`on_eval_before_archive` (function())

Stage called before performance values are written to the archive. Called in `ObjectiveTuning$eval_many()`.

Methods

Public methods:

- `CallbackTuning$clone()`

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

Usage:


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

Arguments:

deep Whether to make a deep clone.

Examples

```
# write archive to disk
callback_tuning("mlr3tuning.backup",
  on_optimization_end = function(callback, context) {
    saveRDS(context$instance$archive, "archive.rds")
  }
)
```

callback_tuning	<i>Create Tuning Callback</i>
-----------------	-------------------------------

Description

Function to create a [CallbackTuning](#). Predefined callbacks are stored in the [dictionary mlr_callbacks](#) and can be retrieved with [clbk\(\)](#).

Tuning callbacks can be called from different stages of tuning process. The stages are prefixed with `on_*`.

```
Start Tuning
  - on_optimization_begin
Start Tuner Batch
  - on_optimizer_before_eval
Start Evaluation
  - on_eval_after_design
  - on_eval_after_benchmark
  - on_eval_before_archive
End Evaluation
  - on_optimizer_after_eval
End Tuner Batch
  - on_result
  - on_optimization_end
End Tuning
```

See also the section on parameters for more information on the stages. A tuning callback works with [bbotk::ContextOptimization](#) and [ContextEval](#).

Usage

```
callback_tuning(
  id,
  label = NA_character_,
  man = NA_character_,
```

```

on_optimization_begin = NULL,
on_optimizer_before_eval = NULL,
on_eval_after_design = NULL,
on_eval_after_benchmark = NULL,
on_eval_before_archive = NULL,
on_optimizer_after_eval = NULL,
on_result = NULL,
on_optimization_end = NULL
)

```

Arguments

id	(character(1)) Identifier for the new instance.
label	(character(1)) Label for the new instance.
man	(character(1)) String in the format [pkg]::[topic] pointing to a manual page for this object. The referenced help package can be opened via method \$help().
on_optimization_begin	(function()) Stage called at the beginning of the optimization. Called in Optimizer\$optimize(). The context available is bbotk::ContextOptimization .
on_optimizer_before_eval	(function()) Stage called after the optimizer proposes points. Called in OptimInstance\$eval_batch(). The context available is bbotk::ContextOptimization .
on_eval_after_design	(function()) Stage called after design is created. Called in ObjectiveTuning\$eval_many(). The context available is ContextEval .
on_eval_after_benchmark	(function()) Stage called after hyperparameter configurations are evaluated. Called in ObjectiveTuning\$eval_many(). The context available is ContextEval .
on_eval_before_archive	(function()) Stage called before performance values are written to the archive. Called in ObjectiveTuning\$eval_many(). The context available is ContextEval .
on_optimizer_after_eval	(function()) Stage called after points are evaluated. Called in OptimInstance\$eval_batch(). The context available is bbotk::ContextOptimization .
on_result	(function()) Stage called after result are written. Called in OptimInstance\$assign_result(). The context available is bbotk::ContextOptimization .

```
on_optimization_end
  (function())
  Stage called at the end of the optimization. Called in Optimizer$optimize().
  The context available is bbotk::ContextOptimization.
```

Details

When implementing a callback, each functions must have two arguments named `callback` and `context`.

A callback can write data to the state (`$state`), e.g. settings that affect the callback itself. Avoid writing large data the state. This can slow down the tuning process when the evaluation of configurations is parallelized.

Tuning callbacks access two different contexts depending on the stage. The stages `on_eval_after_design`, `on_eval_after_benchmark`, `on_eval_before_archive` access [ContextEval](#). This context can be used to customize the evaluation of a batch of hyperparameter configurations. Changes to the state of callback are lost after the evaluation of a batch and changes to the tuning instance or the tuner are not possible. Persistent data should be written to the archive via `$aggregated_performance` (see [ContextEval](#)). The other stages access [ContextOptimization](#). This context can be used to modify the tuning instance, archive, tuner and final result. There are two different contexts because the evaluation can be parallelized i.e. multiple instances of [ContextEval](#) exists on different workers at the same time.

Examples

```
# write archive to disk
callback_tuning("mlr3tuning.backup",
  on_optimization_end = function(callback, context) {
    saveRDS(context$instance$archive, "archive.rds")
  }
)
```

ContextEval

Evaluation Context

Description

The [ContextEval](#) allows [CallbackTunings](#) to access and modify data while a batch of hyperparameter configurations is evaluated. See section on active bindings for a list of modifiable objects. See [callback_tuning\(\)](#) for a list of stages which access [ContextEval](#).

Details

This context is re-created each time a new batch of hyperparameter configurations is evaluated. Changes to `$objective_tuning`, `$design` `$benchmark_result` are discarded after the function is finished. Modification on the data table in `$aggregated_performance` are written to the archive. Any number of columns can be added.

Super class

`mlr3misc::Context` -> ContextEval

Public fields

`objective_tuning` [ObjectiveTuning](#).

Active bindings

`xss` (`list()`)

The hyperparameter configurations of the latest batch. Contains the values on the learner scale i.e. transformations are applied. See `$xdt` in [bbotk::ContextOptimization](#) for the untransformed values.

`design` (`data.table::data.table`)

The benchmark design of the latest batch.

`benchmark_result` (`mlr3::BenchmarkResult`)

The benchmark result of the latest batch.

`aggregated_performance` (`data.table::data.table`)

Aggregated performance scores and training time of the latest batch. This data table is passed to the archive. A callback can add additional columns which are also written to the archive.

Methods**Public methods:**

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

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

Usage:

```
ContextEval$new(objective_tuning)
```

Arguments:

`objective_tuning` [ObjectiveTuning](#).

`id` (`character(1)`)

Identifier for the new callback.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

```
extract_inner_tuning_archives
  Extract Inner Tuning Archives
```

Description

Extract inner tuning archives of nested resampling. Implemented for `mlr3::ResampleResult` and `mlr3::BenchmarkResult`. The function iterates over the `AutoTuner` objects and binds the tuning archives to a `data.table::data.table()`. `AutoTuner` must be initialized with `store_tuning_instance = TRUE` and `mlr3::resample()` or `mlr3::benchmark()` must be called with `store_models = TRUE`.

Usage

```
extract_inner_tuning_archives(
  x,
  unnest = "x_domain",
  exclude_columns = "uhash"
)
```

Arguments

<code>x</code>	(<code>mlr3::ResampleResult</code> <code>mlr3::BenchmarkResult</code>).
<code>unnest</code>	(<code>character()</code>) Transforms list columns to separate columns. By default, <code>x_domain</code> is unnested. Set to <code>NULL</code> if no column should be unnested.
<code>exclude_columns</code>	(<code>character()</code>) Exclude columns from result table. Set to <code>NULL</code> if no column should be excluded.

Value

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

Data structure

The returned data table has the following columns:

- `experiment` (`integer(1)`)
Index, giving the according row number in the original benchmark grid.
- `iteration` (`integer(1)`)
Iteration of the outer resampling.
- One column for each hyperparameter of the search spaces.
- One column for each performance measure.
- `runtime_learners` (`numeric(1)`)
Sum of training and predict times logged in learners per `mlr3::ResampleResult` / evaluation. This does not include potential overhead time.

- `timestamp` (POSIXct)
Time stamp when the evaluation was logged into the archive.
- `batch_nr` (integer(1))
Hyperparameters are evaluated in batches. Each batch has a unique batch number.
- `x_domain` (list())
List of transformed hyperparameter values. By default this column is unnested.
- `x_domain_*` (any)
Separate column for each transformed hyperparameter.
- `resample_result` ([mlr3::ResampleResult](#))
Resample result of the inner resampling.
- `task_id` (character(1)).
- `learner_id` (character(1)).
- `resampling_id` (character(1)).

Examples

```
# Nested Resampling on Palmer Penguins Data Set

learner = lrn("classif.rpart",
  cp = to_tune(1e-04, 1e-1, logscale = TRUE))

# create auto tuner
at = auto_tuner(
  tuner = tnr("random_search"),
  learner = learner,
  resampling = rsmpl("holdout"),
  measure = msr("classif.ce"),
  term_evals = 4)

resampling_outer = rsmpl("cv", folds = 2)
rr = resample(tsk("iris"), at, resampling_outer, store_models = TRUE)

# extract inner archives
extract_inner_tuning_archives(rr)
```

```
extract_inner_tuning_results
```

Extract Inner Tuning Results

Description

Extract inner tuning results of nested resampling. Implemented for [mlr3::ResampleResult](#) and [mlr3::BenchmarkResult](#).

Usage

```
extract_inner_tuning_results(x, tuning_instance, ...)

## S3 method for class 'ResampleResult'
extract_inner_tuning_results(x, tuning_instance = FALSE, ...)

## S3 method for class 'BenchmarkResult'
extract_inner_tuning_results(x, tuning_instance = FALSE, ...)
```

Arguments

```
x                (mlr3::ResampleResult | mlr3::BenchmarkResult).
tuning_instance  (logical(1))
                 If TRUE, tuning instances are added to the table.
...             (any)
                 Additional arguments.
```

Details

The function iterates over the [AutoTuner](#) objects and binds the tuning results to a `data.table::data.table()`. The [AutoTuner](#) must be initialized with `store_tuning_instance = TRUE` and `mlr3::resample()` or `mlr3::benchmark()` must be called with `store_models = TRUE`. Optionally, the tuning instance can be added for each iteration.

Value

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

Data structure

The returned data table has the following columns:

- `experiment` (`integer(1)`)
Index, giving the according row number in the original benchmark grid.
- `iteration` (`integer(1)`)
Iteration of the outer resampling.
- One column for each hyperparameter of the search spaces.
- One column for each performance measure.
- `learner_param_vals` (`list()`)
Hyperparameter values used by the learner. Includes fixed and proposed hyperparameter values.
- `x_domain` (`list()`)
List of transformed hyperparameter values.
- `tuning_instance` (`TuningInstanceSingleCrit` | `TuningInstanceMultiCrit`)
Optionally, tuning instances.
- `task_id` (`character(1)`).

- learner_id(character(1)).
- resampling_id(character(1)).

Examples

```
# Nested Resampling on Palmer Penguins Data Set

learner = lrn("classif.rpart",
  cp = to_tune(1e-04, 1e-1, logscale = TRUE))

# create auto tuner
at = auto_tuner(
  tuner = tnr("random_search"),
  learner = learner,
  resampling = rsmpl("holdout"),
  measure = msr("classif.ce"),
  term_evals = 4)

resampling_outer = rsmpl("cv", folds = 2)
rr = resample(tsk("iris"), at, resampling_outer, store_models = TRUE)

# extract inner results
extract_inner_tuning_results(rr)
```

mlr3tuning.backup

Backup Benchmark Result Callback

Description

This [CallbackTuning](#) writes the `mlr3::BenchmarkResult` after each batch to disk.

Examples

```
clbk("mlr3tuning.backup", path = "backup.rds")

# tune classification tree on the pima data set
instance = tune(
  tuner = tnr("random_search", batch_size = 2),
  task = tsk("pima"),
  learner = lrn("classif.rpart", cp = to_tune(1e-04, 1e-1, logscale = TRUE)),
  resampling = rsmpl("cv", folds = 3),
  measures = msr("classif.ce"),
  term_evals = 4,
  callbacks = clbk("mlr3tuning.backup", path = tempfile(fileext = ".rds"))
)
```

```
mlr3tuning.early_stopping
```

Early Stopping Callback

Description

This [CallbackTuning](#) integrates early stopping into the hyperparameter tuning of an XGBoost learner. Early stopping estimates the optimal number of trees (nrounds) for a given hyperparameter configuration. Since early stopping is performed in each resampling iteration, there are several optimal nrounds values. The callback writes the maximum value to the archive in the max_nrounds column. In the best hyperparameter configuration (instance\$result_learner_param_vals), the value of nrounds is replaced by max_nrounds and early stopping is deactivated.

Details

Currently, the callback does not work with GraphLearners from the package [mlr3pipelines](#). The callback is compatible with the [AutoTuner](#). The final model is fitted with the best hyperparameter configuration and max_nrounds i.e. early stopping is not performed.

Resources

- [gallery post](#) on early stopping with XGBoost.

Examples

```
clbk("mlr3tuning.early_stopping")

if (requireNamespace("mlr3learners") && requireNamespace("xgboost")) {
  library(mlr3learners)

  # activate early stopping on the test set and set search space
  learner = lrn("classif.xgboost",
    eta = to_tune(1e-02, 1e-1, logscale = TRUE),
    early_stopping_rounds = 5,
    nrounds = 100,
    early_stopping_set = "test")

  # tune xgboost on the pima data set
  instance = tune(
    tuner = tnr("random_search"),
    task = tsk("pima"),
    learner = learner,
    resampling = rsmp("cv", folds = 3),
    measures = msr("classif.ce"),
    term_evals = 10,
    callbacks = clbk("mlr3tuning.early_stopping")
  )
}
```

mlr3tuning.measures *Measure Callback*

Description

This `CallbackTuning` scores the hyperparameter configurations on additional measures while tuning. Usually, the configurations can be scored on additional measures after tuning (see [ArchiveTuning](#)). However, if the memory is not sufficient to store the `mlr3::BenchmarkResult`, it is necessary to score the additional measures while tuning. The measures are not taken into account by the tuner.

Examples

```
clbk("mlr3tuning.measures")

# additionally score the configurations on the accuracy measure
instance = tune(
  tuner = tnr("random_search", batch_size = 2),
  task = tsk("pima"),
  learner = lrn("classif.rpart", cp = to_tune(1e-04, 1e-1, logscale = TRUE)),
  resampling = rsmp("cv", folds = 3),
  measures = msr("classif.ce"),
  term_evals = 4,
  callbacks = clbk("mlr3tuning.measures", measures = msr("classif.acc"))
)

# score the configurations on the holdout set
task = tsk("pima")
splits = partition(task, ratio = 0.8)
task$row_roles$use = splits$train
task$row_roles$holdout = splits$test

learner = lrn("classif.rpart", cp = to_tune(1e-04, 1e-1, logscale = TRUE))
learner$predict_sets = c("test", "holdout")

instance = tune(
  tuner = tnr("random_search", batch_size = 2),
  task = task,
  learner = learner,
  resampling = rsmp("cv", folds = 3),
  measures = msr("classif.ce"),
  term_evals = 4,
  callbacks = clbk("mlr3tuning.measures", measures = msr("classif.ce",
    predict_sets = "holdout", id = "classif.ce_holdout"))
)
```

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()`.

Format

`R6::R6Class` object inheriting from `mlr3misc::Dictionary`.

Methods

See `mlr3misc::Dictionary`.

S3 methods

- `as.data.table(dict, ..., objects = FALSE)`
`mlr3misc::Dictionary` -> `data.table::data.table()`
Returns a `data.table::data.table()` with fields "key", "label", "param_classes", "properties" and "packages" as columns. If `objects` is set to `TRUE`, the constructed objects are returned in the list column named `object`.

See Also

Sugar functions: `tnr()`, `tnrs()`

Other Tuner: `mlr_tuners_cmaes`, `mlr_tuners_design_points`, `mlr_tuners_gensa`, `mlr_tuners_grid_search`, `mlr_tuners_irace`, `mlr_tuners_nloptr`, `mlr_tuners_random_search`

Examples

```
as.data.table(mlr_tuners)
mlr_tuners$get("random_search")
tnr("random_search")
```

mlr_tuners_cmaes	<i>Hyperparameter Tuning with Covariance Matrix Adaptation Evolution Strategy</i>
------------------	---

Description

Subclass for Covariance Matrix Adaptation Evolution Strategy (CMA-ES). Calls `adagio::pureCMAES()` from package **adagio**.

Dictionary

This **Tuner** can be instantiated with the associated sugar function `tnr()`:

```
tnr("cmaes")
```

Control Parameters

`start_values` character(1)

Create random start values or based on center of search space? In the latter case, it is the center of the parameters before a trafo is applied.

For the meaning of the control parameters, see `adagio::pureCMAES()`. 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.

Progress Bars

`$optimize()` supports progress bars via the package **progressr** combined with a **Terminator**. Simply wrap the function in `progressr::with_progress()` to enable them. We recommend to use package **progress** as backend; enable with `progressr::handlers("progress")`.

Logging

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

Optimizer

This **Tuner** is based on `bbotk::OptimizerCmaes` which can be applied on any black box optimization problem. See also the documentation of **bbotk**.

Resources

There are several sections about hyperparameter optimization in the **mlr3book**.

- Learn more about **tuners**.

The **gallery** features a collection of case studies and demos about optimization.

- Use the **Hyperband** optimizer with different budget parameters.

Super classes

`mlr3tuning::Tuner` -> `mlr3tuning::TunerFromOptimizer` -> `TunerCmaes`

Methods**Public methods:**

- `TunerCmaes$new()`
- `TunerCmaes$clone()`

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

Usage:

```
TunerCmaes$new()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Source

Hansen N (2016). “The CMA Evolution Strategy: A Tutorial.” 1604.00772.

See Also

Other Tuner: `mlr_tuners_design_points`, `mlr_tuners_gensa`, `mlr_tuners_grid_search`, `mlr_tuners_irace`, `mlr_tuners_nloptr`, `mlr_tuners_random_search`, `mlr_tuners`

Examples

```
# Hyperparameter Optimization

# load learner and set search space
learner = lrn("classif.rpart",
  cp = to_tune(1e-04, 1e-1, logscale = TRUE),
  minsplit = to_tune(p_dbl(2, 128, trafo = as.integer)),
  minbucket = to_tune(p_dbl(1, 64, trafo = as.integer))
)

# run hyperparameter tuning on the Palmer Penguins data set
instance = tune(
  tuner = tnr("cmaes"),
  task = tsk("penguins"),
  learner = learner,
  resampling = rsm("holdout"),
  measure = msr("classif.ce"),
  term_evals = 10)

# best performing hyperparameter configuration
```

```

instance$result

# all evaluated hyperparameter configuration
as.data.table(instance$archive)

# fit final model on complete data set
learner$param_set$values = instance$result_learner_param_vals
learner$train(tsk("penguins"))

```

mlr_tuners_design_points

Hyperparameter Tuning with Design Points

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 with the associated sugar function [tnr\(\)](#):

```
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.

Optimizer

This [Tuner](#) is based on [bbotk::OptimizerDesignPoints](#) which can be applied on any black box optimization problem. See also the documentation of [bbotk](#).

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.

Resources

There are several sections about hyperparameter optimization in the [mlr3book](#).

- Learn more about [tuners](#).

The [gallery](#) features a collection of case studies and demos about optimization.

- Use the [Hyperband](#) optimizer with different budget parameters.

Progress Bars

`$optimize()` supports progress bars via the package [progressr](#) combined with a [Terminator](#). Simply wrap the function in `progressr::with_progress()` to enable them. We recommend to use package [progress](#) as backend; enable with `progressr::handlers("progress")`.

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.

See Also

Package [mlr3hyperband](#) for hyperband tuning.

Other Tuner: [mlr_tuners_cmaes](#), [mlr_tuners_gensa](#), [mlr_tuners_grid_search](#), [mlr_tuners_irace](#), [mlr_tuners_nloptr](#), [mlr_tuners_random_search](#), [mlr_tuners](#)

Examples

```
# Hyperparameter Optimization

# load learner and set search space
learner = lrn("classif.rpart",
  cp = to_tune(1e-04, 1e-1),
  minsplit = to_tune(2, 128),
  minbucket = to_tune(1, 64)
)

# create design
design = mlr3misc::rowwise_table(
  ~cp, ~minsplit, ~minbucket,
  0.1, 2, 64,
  0.01, 64, 32,
  0.001, 128, 1
)

# run hyperparameter tuning on the Palmer Penguins data set
instance = tune(
  tuner = tnr("design_points", design = design),
  task = tsk("penguins"),
  learner = learner,
  resampling = rsmpl("holdout"),
  measure = msr("classif.ce")
)

# best performing hyperparameter configuration
instance$result

# all evaluated hyperparameter configuration
as.data.table(instance$archive)

# fit final model on complete data set
learner$param_set$values = instance$result_learner_param_vals
learner$train(tsk("penguins"))
```

mlr_tuners_gensa

Hyperparameter Tuning with Generalized Simulated Annealing

Description

Subclass for generalized simulated annealing tuning. Calls `GenSA::GenSA()` from package **GenSA**.

Details

In contrast to the `GenSA::GenSA()` defaults, we set `smooth = FALSE` as a default.

Dictionary

This **Tuner** can be instantiated with the associated sugar function `tnr()`:

```
tnr("gensa")
```

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.

Optimizer

This **Tuner** is based on `bbotk::OptimizerGenSA` which can be applied on any black box optimization problem. See also the documentation of **bbotk**.

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.

In contrast to the `GenSA::GenSA()` defaults, we set `trace.mat = FALSE`. Note that `GenSA::GenSA()` uses `smooth = TRUE` as a default. In the case of using this optimizer for Hyperparameter Optimization you may want to set `smooth = FALSE`.

Resources

There are several sections about hyperparameter optimization in the **mlr3book**.

- Learn more about **tuners**.

The **gallery** features a collection of case studies and demos about optimization.

- Use the **Hyperband** optimizer with different budget parameters.

Progress Bars

`$optimize()` supports progress bars via the package **progressr** combined with a [Terminator](#). Simply wrap the function in `progressr::with_progress()` to enable them. We recommend to use package **progress** as backend; enable with `progressr::handlers("progress")`.

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, Stariolo DA (1996). “Generalized simulated annealing.” *Physica A: Statistical Mechanics and its Applications*, **233**(1-2), 395–406. doi: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.

See Also

Other Tuner: [mlr_tuners_cmaes](#), [mlr_tuners_design_points](#), [mlr_tuners_grid_search](#), [mlr_tuners_irace](#), [mlr_tuners_nloptr](#), [mlr_tuners_random_search](#), [mlr_tuners](#)

Examples

```
# Hyperparameter Optimization

# load learner and set search space
learner = lrn("classif.rpart",
  cp = to_tune(1e-04, 1e-1, logscale = TRUE)
)

# run hyperparameter tuning on the Palmer Penguins data set
instance = tune(
```

```

    tuner = tnr("gensa"),
    task = tsk("penguins"),
    learner = learner,
    resampling = rsmp("holdout"),
    measure = msr("classif.ce"),
    term_evals = 10
  )

# best performing hyperparameter configuration
instance$result

# all evaluated hyperparameter configuration
as.data.table(instance$archive)

# fit final model on complete data set
learner$param_set$values = instance$result_learner_param_vals
learner$train(tsk("penguins"))

```

mlr_tuners_grid_search

Hyperparameter Tuning with Grid Search

Description

Subclass for grid search tuning.

Details

The grid is constructed as a Cartesian product over discretized values per parameter, see [paradox::generate_design_grid\(\)](#). If the learner supports hotstarting, the grid is sorted by the hotstart parameter (see also [mlr3::HotstartStack](#)). If not, the points of the grid are evaluated in a random order.

Dictionary

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

```
tnr("grid_search")
```

Control 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.

Progress Bars

`$optimize()` supports progress bars via the package **progressr** combined with a **Terminator**. Simply wrap the function in `progressr::with_progress()` to enable them. We recommend to use package **progress** as backend; enable with `progressr::handlers("progress")`.

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.

Optimizer

This **Tuner** is based on `bbotk::OptimizerGridSearch` which can be applied on any black box optimization problem. See also the documentation of **bbotk**.

Resources

There are several sections about hyperparameter optimization in the **mlr3book**.

- Learn more about **tuners**.

The **gallery** features a collection of case studies and demos about optimization.

- Use the **Hyperband** optimizer with different budget parameters.

Super class

`mlr3tuning::Tuner` -> `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.
```

See Also

Other Tuner: [mlr_tuners_cmaes](#), [mlr_tuners_design_points](#), [mlr_tuners_gensa](#), [mlr_tuners_irace](#), [mlr_tuners_nloptr](#), [mlr_tuners_random_search](#), [mlr_tuners](#)

Examples

```
# Hyperparameter Optimization

# load learner and set search space
learner = lrn("classif.rpart",
  cp = to_tune(1e-04, 1e-1, logscale = TRUE)
)

# run hyperparameter tuning on the Palmer Penguins data set
instance = tune(
  tuner = tnr("grid_search"),
  task = tsk("penguins"),
  learner = learner,
  resampling = rsmpl("holdout"),
  measure = msr("classif.ce"),
  term_evals = 10
)

# best performing hyperparameter configuration
instance$result

# all evaluated hyperparameter configuration
as.data.table(instance$archive)

# fit final model on complete data set
learner$param_set$values = instance$result_learner_param_vals
learner$train(tsk("penguins"))
```

```
mlr_tuners_irace      Hyperparameter Tuning with Iterated Racing.
```

Description

Subclass for iterated racing. Calls `irace::irace()` from package **irace**.

Dictionary

This **Tuner** can be instantiated with the associated sugar function `tnr()`:

```
tnr("irace")
```

Control Parameters

`n_instances` `integer(1)`
 Number of resampling instances.

For the meaning of all other parameters, see `irace::defaultScenario()`. Note that we have removed all control parameters which refer to the termination of the algorithm. Use `TerminatorEvals` instead. Other terminators do not work with `TunerIrace`.

Archive

The `ArchiveTuning` holds the following additional columns:

- `"race"` (`integer(1)`)
Race iteration.
- `"step"` (`integer(1)`)
Step number of race.
- `"instance"` (`integer(1)`)
Identifies resampling instances across races and steps.
- `"configuration"` (`integer(1)`)
Identifies configurations across races and steps.

Result

The tuning result (`instance$result`) is the best performing elite of the final race. The reported performance is the average performance estimated on all used instances.

Progress Bars

`$optimize()` supports progress bars via the package `progressr` combined with a `Terminator`. Simply wrap the function in `progressr::with_progress()` to enable them. We recommend to use package `progress` as backend; enable with `progressr::handlers("progress")`.

Logging

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

Optimizer

This `Tuner` is based on `bbotk::OptimizerIrace` which can be applied on any black box optimization problem. See also the documentation of `bbotk`.

Resources

There are several sections about hyperparameter optimization in the `mlr3book`.

- Learn more about `tuners`.

The `gallery` features a collection of case studies and demos about optimization.

- Use the `Hyperband` optimizer with different budget parameters.

Super classes

`mlr3tuning::Tuner` -> `mlr3tuning::TunerFromOptimizer` -> `TunerIrace`

Methods

Public methods:

- `TunerIrace$new()`
- `TunerIrace$optimize()`
- `TunerIrace$clone()`

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

Usage:

`TunerIrace$new()`

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

Usage:

`TunerIrace$optimize(inst)`

Arguments:

`inst` (`TuningInstanceSingleCrit`).

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

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

Usage:

`TunerIrace$clone(deep = FALSE)`

Arguments:

`deep` Whether to make a deep clone.

Source

Lopez-Ibanez M, Dubois-Lacoste J, Caceres LP, Birattari M, Stuetzle T (2016). “The irace package: Iterated racing for automatic algorithm configuration.” *Operations Research Perspectives*, **3**, 43–58. [doi:10.1016/j.orp.2016.09.002](https://doi.org/10.1016/j.orp.2016.09.002).

See Also

Other Tuner: `mlr_tuners_cmaes`, `mlr_tuners_design_points`, `mlr_tuners_gensa`, `mlr_tuners_grid_search`, `mlr_tuners_nloptr`, `mlr_tuners_random_search`, `mlr_tuners`

Examples

```

# retrieve task
task = tsk("pima")

# load learner and set search space
learner = lrn("classif.rpart", cp = to_tune(1e-04, 1e-1, logscale = TRUE))

# hyperparameter tuning on the pima indians diabetes data set
instance = tune(
  tuner = tnr("irace"),
  task = task,
  learner = learner,
  resampling = rsmpl("holdout"),
  measure = msr("classif.ce"),
  term_evals = 42
)

# best performing hyperparameter configuration
instance$result

# all evaluated hyperparameter configuration
as.data.table(instance$archive)

# fit final model on complete data set
learner$param_set$values = instance$result_learner_param_vals
learner$train(task)

```

mlr_tuners_nloptr

Hyperparameter Tuning with Non-linear Optimization

Description

Subclass for non-linear optimization (NLOpt). 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 with the associated sugar function `tnr()`:

```
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.

Optimizer

This **Tuner** is based on `bbotk::OptimizerNloptr` which can be applied on any black box optimization problem. See also the documentation of **bbotk**.

Parameters

`algorithm` character(1)

`eval_g_ineq` function()

`xtol_rel` numeric(1)

`xtol_abs` numeric(1)

`ftol_rel` numeric(1)

`ftol_abs` numeric(1)

`start_values` character(1)

Create random start values or based on center of search space? In the latter case, it is the center of the parameters before a trafo is applied.

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`.

Resources

There are several sections about hyperparameter optimization in the **mlr3book**.

- Learn more about **tuners**.

The **gallery** features a collection of case studies and demos about optimization.

- Use the **Hyperband** optimizer with different budget parameters.

Progress Bars

`$optimize()` supports progress bars via the package **progressr** combined with a **Terminator**. Simply wrap the function in `progressr::with_progress()` to enable them. We recommend to use package **progress** as backend; enable with `progressr::handlers("progress")`.

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, G S (2020). “The NLOpt nonlinear-optimization package.” <https://github.com/stevengj/nlopt>.

See Also

Other Tuner: [mlr_tuners_cmaes](#), [mlr_tuners_design_points](#), [mlr_tuners_gensa](#), [mlr_tuners_grid_search](#), [mlr_tuners_irace](#), [mlr_tuners_random_search](#), [mlr_tuners](#)

Examples

```
# Hyperparameter Optimization

# load learner and set search space
learner = lrn("classif.rpart",
  cp = to_tune(1e-04, 1e-1, logscale = TRUE)
)

# run hyperparameter tuning on the Palmer Penguins data set
instance = tune(
  tuner = tnr("nloptr", algorithm = "NLOPT_LN_BOBYQA"),
  task = tsk("penguins"),
  learner = learner,
  resampling = rsmpl("holdout"),
  measure = msr("classif.ce")
)

# best performing hyperparameter configuration
instance$result

# all evaluated hyperparameter configuration
as.data.table(instance$archive)
```

```
# fit final model on complete data set
learner$param_set$values = instance$result_learner_param_vals
learner$train(tsk("penguins"))
```

mlr_tuners_random_search

Hyperparameter Tuning with Random Search

Description

Subclass for random search tuning.

Details

The random points are sampled by `paradox::generate_design_random()`.

Dictionary

This **Tuner** can be instantiated with the associated sugar function `tnr()`:

```
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.

Optimizer

This **Tuner** is based on `bbotk::OptimizerRandomSearch` which can be applied on any black box optimization problem. See also the documentation of **bbotk**.

Parameters

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

Resources

There are several sections about hyperparameter optimization in the [mlr3book](#).

- Learn more about [tuners](#).

The [gallery](#) features a collection of case studies and demos about optimization.

- Use the [Hyperband](#) optimizer with different budget parameters.

Progress Bars

`$optimize()` supports progress bars via the package [progressr](#) combined with a [Terminator](#). Simply wrap the function in `progressr::with_progress()` to enable them. We recommend to use package [progress](#) as backend; enable with `progressr::handlers("progress")`.

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. <https://jmlr.csail.mit.edu/papers/v13/bergstra12a.html>.

See Also

Package [mlr3hyperband](#) for hyperband tuning.

Other Tuner: [mlr_tuners_cmaes](#), [mlr_tuners_design_points](#), [mlr_tuners_gensa](#), [mlr_tuners_grid_search](#), [mlr_tuners_irace](#), [mlr_tuners_nloptr](#), [mlr_tuners](#)

Examples

```

# Hyperparameter Optimization

# load learner and set search space
learner = lrn("classif.rpart",
  cp = to_tune(1e-04, 1e-1, logscale = TRUE)
)

# run hyperparameter tuning on the Palmer Penguins data set
instance = tune(
  tuner = tnr("random_search"),
  task = tsk("penguins"),
  learner = learner,
  resampling = rsmpl("holdout"),
  measure = msr("classif.ce"),
  term_evals = 10
)

# best performing hyperparameter configuration
instance$result

# all evaluated hyperparameter configuration
as.data.table(instance$archive)

# fit final model on complete data set
learner$param_set$values = instance$result_learner_param_vals
learner$train(tsk("penguins"))

```

ObjectiveTuning

Class for Tuning Objective

Description

Stores the objective function that estimates the performance of hyperparameter configurations. This class is usually constructed internally by the [TuningInstanceSingleCrit](#) or [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_benchmark_result (logical(1)).
 archive ([ArchiveTuning](#)).
 hotstart_stack ([mlr3::HotstartStack](#)).
 allow_hotstart (logical(1)).
 keep_hotstart_stack (logical(1)).
 callbacks (List of [CallbackTunings](#)).

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_benchmark_result = TRUE,
  store_models = FALSE,
  check_values = TRUE,
  allow_hotstart = FALSE,
  keep_hotstart_stack = FALSE,
  archive = NULL,
  callbacks = list()
)
```

Arguments:

task ([mlr3::Task](#))

Task to operate on.

learner ([mlr3::Learner](#))

Learner to tune.

resampling ([mlr3::Resampling](#))

Resampling that is used to evaluate the performance of the hyperparameter configurations. Uninstantiated resamplings are instantiated during construction so that all configurations are evaluated on the same data splits. Already instantiated resamplings are kept unchanged. Specialized [Tuner](#) change the resampling e.g. to evaluate a hyperparameter configuration on different data splits. This field, however, always returns the resampling passed in construction.

measures (list of [mlr3::Measure](#))

Measures to optimize.

store_benchmark_result (logical(1))

If TRUE (default), store resample result of evaluated hyperparameter configurations in archive as [mlr3::BenchmarkResult](#).

`store_models` (logical(1))
 If TRUE, fitted models are stored in the benchmark result (`archive$benchmark_result`). If `store_benchmark_result = FALSE`, models are only stored temporarily and not accessible after the tuning. This combination is needed for measures that require a model.

`check_values` (logical(1))
 If TRUE, hyperparameter values are checked before evaluation and performance scores after. If FALSE (default), values are unchecked but computational overhead is reduced.

`allow_hotstart` (logical(1))
 Allow to hotstart learners with previously fitted models. See also [mlr3::HotstartStack](#). The learner must support hotstarting. Sets `store_models = TRUE`.

`keep_hotstart_stack` (logical(1))
 If TRUE, [mlr3::HotstartStack](#) is kept in `$objective$hotstart_stack` after tuning.

`archive` ([ArchiveTuning](#))
 Reference to archive of [TuningInstanceSingleCrit](#) | [TuningInstanceMultiCrit](#). If NULL (default), benchmark result and models cannot be stored.

`callbacks` (list of [CallbackTuning](#))
 List of callbacks.

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

Function to construct a [TuningInstanceSingleCrit](#) or [TuningInstanceMultiCrit](#).

Usage

```
ti(
  task,
  learner,
  resampling,
  measures = NULL,
  terminator,
  search_space = NULL,
  store_benchmark_result = TRUE,
  store_models = FALSE,
  check_values = FALSE,
  allow_hotstart = FALSE,
  keep_hotstart_stack = FALSE,
  evaluate_default = FALSE,
  callbacks = list()
)
```

Arguments

task	(mlr3::Task) Task to operate on.
learner	(mlr3::Learner) Learner to tune.
resampling	(mlr3::Resampling) Resampling that is used to evaluate the performance of the hyperparameter configurations. Uninstantiated resamplings are instantiated during construction so that all configurations are evaluated on the same data splits. Already instantiated resamplings are kept unchanged. Specialized Tuner change the resampling e.g. to evaluate a hyperparameter configuration on different data splits. This field, however, always returns the resampling passed in construction.
measures	(mlr3::Measure or list of mlr3::Measure) A single measure creates a TuningInstanceSingleCrit and multiple measures a TuningInstanceMultiCrit . If NULL, default measure is used.
terminator	(Terminator) Stop criterion of the tuning process.
search_space	(paradox::ParamSet) Hyperparameter search space. If NULL (default), the search space is constructed from the TuneToken of the learner's parameter set (learner\$param_set).
store_benchmark_result	(logical(1)) If TRUE (default), store resample result of evaluated hyperparameter configurations in archive as mlr3::BenchmarkResult .
store_models	(logical(1)) If TRUE, fitted models are stored in the benchmark result (archive\$benchmark_result). If store_benchmark_result = FALSE, models are only stored temporarily and not accessible after the tuning. This combination is needed for measures that require a model.
check_values	(logical(1)) If TRUE, hyperparameter values are checked before evaluation and performance scores after. If FALSE (default), values are unchecked but computational overhead is reduced.
allow_hotstart	(logical(1)) Allow to hotstart learners with previously fitted models. See also mlr3::HotstartStack . The learner must support hotstarting. Sets store_models = TRUE.
keep_hotstart_stack	(logical(1)) If TRUE, mlr3::HotstartStack is kept in \$objective\$hotstart_stack after tuning.
evaluate_default	(logical(1)) If TRUE, learner is evaluated with hyperparameters set to their default values at the start of the optimization.
callbacks	(list of CallbackTuning) List of callbacks.

Resources

There are several sections about hyperparameter optimization in the [mlr3book](#).

- Getting started with [hyperparameter optimization](#).
- [Tune](#) a simple classification tree on the Sonar data set.
- Learn about [tuning spaces](#).

The [gallery](#) features a collection of case studies and demos about optimization.

- Learn more advanced methods with the [practical tuning series](#).
- Simultaneously optimize hyperparameters and use [early stopping](#) with XGBoost.
- Make us of proven [search space](#).
- Learn about [hotstarting](#) models.
- Run the [default hyperparameter configuration](#) of learners as a baseline.

Default Measures

If no measure is passed, the default measure is used. The default measure depends on the task type.

Task	Default Measure	Package
"classif"	"classif.ce"	mlr3
"regr"	"regr.mse"	mlr3
"surv"	"surv.cindex"	mlr3proba
"dens"	"dens.logloss"	mlr3proba
"classif_st"	"classif.ce"	mlr3spatial
"regr_st"	"regr.mse"	mlr3spatial
"clust"	"clust.dunn"	mlr3cluster

Examples

```
# Hyperparameter optimization on the Palmer Penguins data set
task = tsk("penguins")

# Load learner and set search space
learner = lrn("classif.rpart",
  cp = to_tune(1e-04, 1e-1, logscale = TRUE)
)

# Construct tuning instance
instance = ti(
  task = task,
  learner = learner,
  resampling = rsmpl("cv", folds = 3),
  measures = msr("classif.ce"),
  terminator = trm("evals", n_evals = 4)
)

# Choose optimization algorithm
```

```

tuner = tnr("random_search", batch_size = 2)

# Run tuning
tuner$optimize(instance)

# Set optimal hyperparameter configuration to learner
learner$param_set$values = instance$result_learner_param_vals

# Train the learner on the full data set
learner$train(task)

# Inspect all evaluated configurations
as.data.table(instance$archive)

```

tnr

*Syntactic Sugar for Tuning Objects Construction***Description**

Functions to retrieve objects, set parameters and assign to fields in one go. Relies on `mlr3misc::dictionary_sugar_get()` to extract objects from the respective `mlr3misc::Dictionary`:

- `tnr()` for a **Tuner** from `mlr_tuners`.
- `tnrs()` for a list of **Tuners** from `mlr_tuners`.
- `trm()` for a **Terminator** from `mlr_terminators`.
- `trms()` for a list of **Terminators** from `mlr_terminators`.

Usage

```
tnr(.key, ...)
```

```
tnrs(.keys, ...)
```

Arguments

<code>.key</code>	(character(1)) Key passed to the respective <code>dictionary</code> to retrieve the object.
<code>...</code>	(named list()) Named arguments passed to the constructor, to be set as parameters in the <code>paradox::ParamSet</code> , or to be set as public field. See <code>mlr3misc::dictionary_sugar_get()</code> for more details.
<code>.keys</code>	(character()) Keys passed to the respective <code>dictionary</code> to retrieve multiple objects.

Value

`R6::R6Class` object of the respective type, or a list of `R6::R6Class` objects for the plural versions.

Examples

```
# random search tuner with batch size of 5
tnr("random_search", batch_size = 5)

# run time terminator with 20 seconds
trm("run_time", secs = 20)
```

tune

Function for Tuning a Learner

Description

Function to tune a `mlr3::Learner`. The function internally creates a `TuningInstanceSingleCrit` or `TuningInstanceMultiCrit` which describe the tuning problem. It executes the tuning with the `Tuner` (tuner) and returns the result with the tuning instance (`$result`). The `ArchiveTuning` (`$archive`) stores all evaluated hyperparameter configurations and performance scores.

Usage

```
tune(
  tuner,
  task,
  learner,
  resampling,
  measures = NULL,
  term_evals = NULL,
  term_time = NULL,
  terminator = NULL,
  search_space = NULL,
  store_benchmark_result = TRUE,
  store_models = FALSE,
  check_values = FALSE,
  allow_hotstart = FALSE,
  keep_hotstart_stack = FALSE,
  evaluate_default = FALSE,
  callbacks = list(),
  method
)
```

Arguments

tuner	(Tuner) Optimization algorithm.
task	(mlr3::Task) Task to operate on.
learner	(mlr3::Learner) Learner to tune.

resampling	(mlr3::Resampling) Resampling that is used to evaluate the performance of the hyperparameter configurations. Uninstantiated resamplings are instantiated during construction so that all configurations are evaluated on the same data splits. Already instantiated resamplings are kept unchanged. Specialized Tuner change the resampling e.g. to evaluate a hyperparameter configuration on different data splits. This field, however, always returns the resampling passed in construction.
measures	(mlr3::Measure or list of mlr3::Measure) A single measure creates a TuningInstanceSingleCrit and multiple measures a TuningInstanceMultiCrit . If NULL, default measure is used.
term_evals	(integer(1)) Number of allowed evaluations. Ignored if terminator is passed.
term_time	(integer(1)) Maximum allowed time in seconds. Ignored if terminator is passed.
terminator	(Terminator) Stop criterion of the tuning process.
search_space	(paradox::ParamSet) Hyperparameter search space. If NULL (default), the search space is constructed from the TuneToken of the learner's parameter set (<code>learner\$param_set</code>).
store_benchmark_result	(logical(1)) If TRUE (default), store resample result of evaluated hyperparameter configurations in archive as mlr3::BenchmarkResult .
store_models	(logical(1)) If TRUE, fitted models are stored in the benchmark result (<code>archive\$benchmark_result</code>). If <code>store_benchmark_result = FALSE</code> , models are only stored temporarily and not accessible after the tuning. This combination is needed for measures that require a model.
check_values	(logical(1)) If TRUE, hyperparameter values are checked before evaluation and performance scores after. If FALSE (default), values are unchecked but computational overhead is reduced.
allow_hotstart	(logical(1)) Allow to hotstart learners with previously fitted models. See also mlr3::HotstartStack . The learner must support hotstarting. Sets <code>store_models = TRUE</code> .
keep_hotstart_stack	(logical(1)) If TRUE, mlr3::HotstartStack is kept in <code>\$objective\$hotstart_stack</code> after tuning.
evaluate_default	(logical(1)) If TRUE, learner is evaluated with hyperparameters set to their default values at the start of the optimization.
callbacks	(list of CallbackTuning) List of callbacks.

method (character(1))
Deprecated. Use tuner instead.

Details

The `mlr3::Task`, `mlr3::Learner`, `mlr3::Resampling`, `mlr3::Measure` and `Terminator` are used to construct a `TuningInstanceSingleCrit`. If multiple performance `Measures` are supplied, a `TuningInstanceMultiCrit` is created. The parameter `term_evals` and `term_time` are shortcuts to create a `Terminator`. If both parameters are passed, a `TerminatorCombo` is constructed. For other `Terminators`, pass one with `terminator`. If no termination criterion is needed, set `term_evals`, `term_time` and `terminator` to `NULL`. The search space is created from `paradox::TuneToken` or is supplied by `search_space`.

Value

`TuningInstanceSingleCrit` | `TuningInstanceMultiCrit`

Resources

There are several sections about hyperparameter optimization in the [mlr3book](#).

- Simplify tuning with the `tune()` function.
- Learn about [tuning spaces](#).

The [gallery](#) features a collection of case studies and demos about optimization.

- Optimize an rpart classification tree with only a [few lines of code](#).
- Tune an XGBoost model with [early stopping](#).
- Make us of proven [search space](#).
- Learn about [hotstarting](#) models.

Default Measures

If no measure is passed, the default measure is used. The default measure depends on the task type.

Task	Default Measure	Package
"classif"	"classif.ce"	mlr3
"regr"	"regr.mse"	mlr3
"surv"	"surv.cindex"	mlr3proba
"dens"	"dens.logloss"	mlr3proba
"classif_st"	"classif.ce"	mlr3spatial
"regr_st"	"regr.mse"	mlr3spatial
"clust"	"clust.dunn"	mlr3cluster

Analysis

For analyzing the tuning results, it is recommended to pass the `ArchiveTuning` to `as.data.table()`. The returned data table is joined with the benchmark result which adds the `mlr3::ResampleResult`

for each hyperparameter evaluation.

The archive provides various getters (e.g. `$learners()`) to ease the access. All getters extract by position (`i`) or unique hash (`uhash`). For a complete list of all getters see the methods section.

The benchmark result (`$benchmark_result`) allows to score the hyperparameter configurations again on a different measure. Alternatively, measures can be supplied to `as.data.table()`.

The **mlr3viz** package provides visualizations for tuning results.

Examples

```
# Hyperparameter optimization on the Palmer Penguins data set
task = tsk("pima")

# Load learner and set search space
learner = lrn("classif.rpart",
  cp = to_tune(1e-04, 1e-1, logscale = TRUE)
)

# Run tuning
instance = tune(
  tuner = tnr("random_search", batch_size = 2),
  task = tsk("pima"),
  learner = learner,
  resampling = rsmpl("holdout"),
  measures = msr("classif.ce"),
  terminator = trm("evals", n_evals = 4)
)

# Set optimal hyperparameter configuration to learner
learner$param_set$values = instance$result_learner_param_vals

# Train the learner on the full data set
learner$train(task)

# Inspect all evaluated configurations
as.data.table(instance$archive)
```

Tuner

Class for Tuning Algorithms

Description

The **Tuner** implements the optimization algorithm.

Details

Tuner is an abstract base class that implements the base functionality each tuner must provide. A subclass is implemented in the following way:

- Inherit from **Tuner**.

- Specify the private abstract method `$.optimize()` and use it to call into your optimizer.
- You need to call `instance$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$archive`.
- Before the batch evaluation, the [bbotk::Terminator](#) is checked, and if it is positive, an exception of class `"terminated_error"` is generated. In the later case the current batch of evaluations is still stored in `instance`, but the numeric scores are not sent back to the handling optimizer as it has lost execution control.
- After such an exception was caught we select the best configuration from `instance$archive` and return it.
- Note that therefore more points than specified by the [bbotk::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.

Private Methods

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

Resources

There are several sections about hyperparameter optimization in the [mlr3book](#).

- Learn more about [tuners](#).

The [gallery](#) features a collection of case studies and demos about optimization.

- Use the [Hyperband](#) optimizer with different budget parameters.

Extension Packages

Additional tuners are provided by the following packages.

- [mlr3hyperband](#) adds the Hyperband and Successive Halving algorithm.
- [mlr3mbo](#) adds Bayesian optimization methods.

Public fields

`id (character(1))`
Identifier of the object. Used in tables, plot and text output.

Active bindings

- `param_set` ([paradox::ParamSet](#))
Set of control parameters.
- `param_classes` (`character()`)
Supported parameter classes for learner hyperparameters that the tuner can optimize. Sub-classes of [paradox::Param](#).
- `properties` (`character()`)
Set of properties of the tuner. Must be a subset of `mlr_reflections$tuner_properties`.
- `packages` (`character()`)
Set of required packages. Note that these packages will be loaded via `requireNamespace()`, and are not attached.
- `label` (`character(1)`)
Label for this object. Can be used in tables, plot and text output instead of the ID.
- `man` (`character(1)`)
String in the format `[pkg]::[topic]` pointing to a manual page for this object. The referenced help package can be opened via method `$help()`.

Methods**Public methods:**

- [Tuner\\$new\(\)](#)
- [Tuner\\$format\(\)](#)
- [Tuner\\$print\(\)](#)
- [Tuner\\$help\(\)](#)
- [Tuner\\$optimize\(\)](#)
- [Tuner\\$clone\(\)](#)

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

Usage:

```
Tuner$new(
  id = "tuner",
  param_set,
  param_classes,
  properties,
  packages = character(),
  label = NA_character_,
  man = NA_character_
)
```

Arguments:

- `id` (`character(1)`)
Identifier for the new instance.
- `param_set` ([paradox::ParamSet](#))
Set of control parameters.

`param_classes` (character())
Supported parameter classes for learner hyperparameters that the tuner can optimize. Sub-classes of [paradox::Param](#).

`properties` (character())
Set of properties of the tuner. Must be a subset of `mlr_reflections$tuner_properties`.

`packages` (character())
Set of required packages. Note that these packages will be loaded via `requireNamespace()`, and are not attached.

`label` (character(1))
Label for this object. Can be used in tables, plot and text output instead of the ID.

`man` (character(1))
String in the format `[pkg]::[topic]` pointing to a manual page for this object. The referenced help package can be opened via method `$help()`.

Method `format()`: Helper for print outputs.

Usage:

`Tuner$format(...)`

Arguments:

... (ignored).

Returns: (character()).

Method `print()`: Print method.

Usage:

`Tuner$print()`

Returns: (character()).

Method `help()`: Opens the corresponding help page referenced by field `$man`.

Usage:

`Tuner$help()`

Method `optimize()`: Performs the tuning on a [TuningInstanceSingleCrit](#) or [TuningInstanceMultiCrit](#) until termination. The single evaluations will be written into the [ArchiveTuning](#) that resides in the [TuningInstanceSingleCrit/TuningInstanceMultiCrit](#). The result will be written into the instance object.

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.

tune_nested	<i>Function for Nested Resampling</i>
-------------	---------------------------------------

Description

Function to conduct nested resampling.

Usage

```
tune_nested(  
  tuner,  
  task,  
  learner,  
  inner_resampling,  
  outer_resampling,  
  measure = NULL,  
  term_evals = NULL,  
  term_time = NULL,  
  terminator = NULL,  
  search_space = NULL,  
  store_tuning_instance = TRUE,  
  store_benchmark_result = TRUE,  
  store_models = FALSE,  
  check_values = FALSE,  
  allow_hotstart = FALSE,  
  keep_hotstart_stack = FALSE,  
  evaluate_default = FALSE,  
  callbacks = list(),  
  method  
)
```

Arguments

tuner	(Tuner) Optimization algorithm.
task	(mlr3::Task) Task to operate on.
learner	(mlr3::Learner) Learner to tune.
inner_resampling	(mlr3::Resampling) Resampling used for the inner loop.
outer_resampling	(mlr3::Resampling) Resampling used for the outer loop.

measure	(mlr3::Measure) Measure to optimize. If NULL, default measure is used.
term_evals	(integer(1)) Number of allowed evaluations. Ignored if terminator is passed.
term_time	(integer(1)) Maximum allowed time in seconds. Ignored if terminator is passed.
terminator	(Terminator) Stop criterion of the tuning process.
search_space	(paradox::ParamSet) Hyperparameter search space. If NULL (default), the search space is constructed from the TuneToken of the learner's parameter set (learner\$param_set).
store_tuning_instance	(logical(1)) If TRUE (default), stores the internally created TuningInstanceSingleCrit with all intermediate results in slot \$tuning_instance.
store_benchmark_result	(logical(1)) If TRUE (default), store resample result of evaluated hyperparameter configurations in archive as mlr3::BenchmarkResult .
store_models	(logical(1)) If TRUE, fitted models are stored in the benchmark result (archive\$benchmark_result). If store_benchmark_result = FALSE, models are only stored temporarily and not accessible after the tuning. This combination is needed for measures that require a model.
check_values	(logical(1)) If TRUE, hyperparameter values are checked before evaluation and performance scores after. If FALSE (default), values are unchecked but computational overhead is reduced.
allow_hotstart	(logical(1)) Allow to hotstart learners with previously fitted models. See also mlr3::HotstartStack . The learner must support hotstarting. Sets store_models = TRUE.
keep_hotstart_stack	(logical(1)) If TRUE, mlr3::HotstartStack is kept in \$objective\$hotstart_stack after tuning.
evaluate_default	(logical(1)) If TRUE, learner is evaluated with hyperparameters set to their default values at the start of the optimization.
callbacks	(list of CallbackTuning) List of callbacks.
method	(character(1)) Deprecated. Use tuner instead.

Value[mlr3::ResampleResult](#)

Examples

```
# Nested resampling on Palmer Penguins data set
rr = tune_nested(
  tuner = tnr("random_search", batch_size = 2),
  task = tsk("penguins"),
  learner = lrn("classif.rpart", cp = to_tune(1e-04, 1e-1, logscale = TRUE)),
  inner_resampling = rsmp("holdout"),
  outer_resampling = rsmp("cv", folds = 2),
  measure = msr("classif.ce"),
  term_evals = 2)

# Performance scores estimated on the outer resampling
rr$score()

# Unbiased performance of the final model trained on the full data set
rr$aggregate()
```

TuningInstanceMultiCrit

Class for Multi Criteria Tuning

Description

The [TuningInstanceMultiCrit](#) specifies a tuning problem for [Tuners](#). The function [ti\(\)](#) creates a [TuningInstanceMultiCrit](#) and the function [tune\(\)](#) creates an instance internally.

Details

The instance contains an [ObjectiveTuning](#) object that encodes the black box objective function a [Tuner](#) has to optimize. The instance allows the basic operations of querying the objective at design points ([\\$eval_batch\(\)](#)). This operation is usually done by the [Tuner](#). Evaluations of hyperparameter configurations are performed in batches by calling [mlr3::benchmark\(\)](#) internally. The evaluated hyperparameter configurations are stored in the [Archive](#) ([\\$archive](#)). 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](#).

Resources

There are several sections about hyperparameter optimization in the [mlr3book](#).

- Learn about [multi-objective optimization](#).

The [gallery](#) features a collection of case studies and demos about optimization.

Analysis

For analyzing the tuning results, it is recommended to pass the [ArchiveTuning](#) to `as.data.table()`. The returned data table is joined with the benchmark result which adds the [mlr3::ResampleResult](#) for each hyperparameter evaluation.

The archive provides various getters (e.g. `$learners()`) to ease the access. All getters extract by position (`i`) or unique hash (`uhash`). For a complete list of all getters see the methods section.

The benchmark result (`$benchmark_result`) allows to score the hyperparameter configurations again on a different measure. Alternatively, measures can be supplied to `as.data.table()`.

The [mlr3viz](#) package provides visualizations for tuning results.

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.

Usage:

```
TuningInstanceMultiCrit$new(
  task,
  learner,
  resampling,
  measures,
  terminator,
  search_space = NULL,
  store_benchmark_result = TRUE,
  store_models = FALSE,
  check_values = FALSE,
  allow_hotstart = FALSE,
  keep_hotstart_stack = FALSE,
  evaluate_default = FALSE,
  callbacks = list()
)
```

Arguments:

```
task (mlr3::Task)
  Task to operate on.
```

learner ([mlr3::Learner](#))
 Learner to tune.

resampling ([mlr3::Resampling](#))
 Resampling that is used to evaluate the performance of the hyperparameter configurations. Uninstantiated resamplings are instantiated during construction so that all configurations are evaluated on the same data splits. Already instantiated resamplings are kept unchanged. Specialized [Tuner](#) change the resampling e.g. to evaluate a hyperparameter configuration on different data splits. This field, however, always returns the resampling passed in construction.

measures (list of [mlr3::Measure](#))
 Measures to optimize.

terminator ([Terminator](#))
 Stop criterion of the tuning process.

search_space ([paradox::ParamSet](#))
 Hyperparameter search space. If NULL (default), the search space is constructed from the [TuneToken](#) of the learner's parameter set (learner\$param_set).

store_benchmark_result (logical(1))
 If TRUE (default), store resample result of evaluated hyperparameter configurations in archive as [mlr3::BenchmarkResult](#).

store_models (logical(1))
 If TRUE, fitted models are stored in the benchmark result (archive\$benchmark_result). If store_benchmark_result = FALSE, models are only stored temporarily and not accessible after the tuning. This combination is needed for measures that require a model.

check_values (logical(1))
 If TRUE, hyperparameter values are checked before evaluation and performance scores after. If FALSE (default), values are unchecked but computational overhead is reduced.

allow_hotstart (logical(1))
 Allow to hotstart learners with previously fitted models. See also [mlr3::HotstartStack](#). The learner must support hotstarting. Sets store_models = TRUE.

keep_hotstart_stack (logical(1))
 If TRUE, [mlr3::HotstartStack](#) is kept in \$objective\$hotstart_stack after tuning.

evaluate_default (logical(1))
 If TRUE, learner is evaluated with hyperparameters set to their default values at the start of the optimization.

callbacks (list of [CallbackTuning](#))
 List of callbacks.

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()`)

Hyperparameter values as `data.table::data.table()`. Each row is one configuration. Contains values in the search space. Can contain additional columns for extra information.

```
ydt (data.table::data.table())
  Optimal outcomes, e.g. the Pareto front.
learner_param_vals (List of named list(s)
  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.

Examples

```
# Hyperparameter optimization on the Palmer Penguins data set
task = tsk("penguins")

# Load learner and set search space
learner = lrn("classif.rpart",
  cp = to_tune(1e-04, 1e-1, logscale = TRUE)
)

# Construct tuning instance
instance = ti(
  task = task,
  learner = learner,
  resampling = rsmpl("cv", folds = 3),
  measures = msrs(c("classif.ce", "time_train")),
  terminator = trm("evals", n_evals = 4)
)

# Choose optimization algorithm
tuner = tnr("random_search", batch_size = 2)

# Run tuning
tuner$optimize(instance)

# Optimal hyperparameter configurations
instance$result

# Inspect all evaluated configurations
as.data.table(instance$archive)
```

TuningInstanceSingleCrit

Class for Single Criterion Tuning

Description

The [TuningInstanceSingleCrit](#) specifies a tuning problem for [Tuners](#). The function `ti()` creates a [TuningInstanceSingleCrit](#) and the function `tune()` creates an instance internally.

Details

The instance contains an [ObjectiveTuning](#) object that encodes the black box objective function a [Tuner](#) has to optimize. The instance allows the basic operations of querying the objective at design points (`$eval_batch()`). This operation is usually done by the [Tuner](#). Evaluations of hyperparameter configurations are performed in batches by calling `mlr3::benchmark()` internally. The evaluated hyperparameter configurations are stored in the [Archive](#) (`$archive`). 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`.

Default Measures

If no measure is passed, the default measure is used. The default measure depends on the task type.

Task	Default Measure	Package
"classif"	"classif.ce"	mlr3
"regr"	"regr.mse"	mlr3
"surv"	"surv.cindex"	mlr3proba
"dens"	"dens.logloss"	mlr3proba
"classif_st"	"classif.ce"	mlr3spatial
"regr_st"	"regr.mse"	mlr3spatial
"clust"	"clust.dunn"	mlr3cluster

Resources

There are several sections about hyperparameter optimization in the [mlr3book](#).

- Getting started with [hyperparameter optimization](#).
- [Tune](#) a simple classification tree on the Sonar data set.
- Learn about [tuning spaces](#).

The [gallery](#) features a collection of case studies and demos about optimization.

- Learn more advanced methods with the [practical tuning series](#).
- Simultaneously optimize hyperparameters and use [early stopping](#) with XGBoost.
- Make us of proven [search space](#).
- Learn about [hotstarting](#) models.
- Run the [default hyperparameter configuration](#) of learners as a baseline.

Extension Packages

mlr3tuning is extended by the following packages.

- [mlr3tuningspaces](#) is a collection of search spaces from scientific articles for commonly used learners.
- [mlr3hyperband](#) adds the Hyperband and Successive Halving algorithm.
- [mlr3mbo](#) adds Bayesian optimization methods.

Analysis

For analyzing the tuning results, it is recommended to pass the [ArchiveTuning](#) to `as.data.table()`. The returned data table is joined with the benchmark result which adds the [mlr3::ResampleResult](#) for each hyperparameter evaluation.

The archive provides various getters (e.g. `$learners()`) to ease the access. All getters extract by position (`i`) or unique hash (`uhash`). For a complete list of all getters see the methods section.

The benchmark result (`$benchmark_result`) allows to score the hyperparameter configurations again on a different measure. Alternatively, measures can be supplied to `as.data.table()`.

The [mlr3viz](#) package provides visualizations for tuning results.

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.

Usage:

```
TuningInstanceSingleCrit$new(
  task,
  learner,
  resampling,
  measure = NULL,
  terminator,
  search_space = NULL,
  store_benchmark_result = TRUE,
  store_models = FALSE,
  check_values = FALSE,
  allow_hotstart = FALSE,
  keep_hotstart_stack = FALSE,
  evaluate_default = FALSE,
  callbacks = list()
)
```

Arguments:

```
task (mlr3::Task)
  Task to operate on.
```

learner ([mlr3::Learner](#))
 Learner to tune.

resampling ([mlr3::Resampling](#))
 Resampling that is used to evaluate the performance of the hyperparameter configurations. Uninstantiated resamplings are instantiated during construction so that all configurations are evaluated on the same data splits. Already instantiated resamplings are kept unchanged. Specialized [Tuner](#) change the resampling e.g. to evaluate a hyperparameter configuration on different data splits. This field, however, always returns the resampling passed in construction.

measure ([mlr3::Measure](#))
 Measure to optimize. If NULL, default measure is used.

terminator ([Terminator](#))
 Stop criterion of the tuning process.

search_space ([paradox::ParamSet](#))
 Hyperparameter search space. If NULL (default), the search space is constructed from the [TuneToken](#) of the learner's parameter set (learner\$param_set).

store_benchmark_result (logical(1))
 If TRUE (default), store resample result of evaluated hyperparameter configurations in archive as [mlr3::BenchmarkResult](#).

store_models (logical(1))
 If TRUE, fitted models are stored in the benchmark result (archive\$benchmark_result). If store_benchmark_result = FALSE, models are only stored temporarily and not accessible after the tuning. This combination is needed for measures that require a model.

check_values (logical(1))
 If TRUE, hyperparameter values are checked before evaluation and performance scores after. If FALSE (default), values are unchecked but computational overhead is reduced.

allow_hotstart (logical(1))
 Allow to hotstart learners with previously fitted models. See also [mlr3::HotstartStack](#). The learner must support hotstarting. Sets store_models = TRUE.

keep_hotstart_stack (logical(1))
 If TRUE, [mlr3::HotstartStack](#) is kept in \$objective\$hotstart_stack after tuning.

evaluate_default (logical(1))
 If TRUE, learner is evaluated with hyperparameters set to their default values at the start of the optimization.

callbacks (list of [CallbackTuning](#))
 List of callbacks.

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()`)

Hyperparameter values as `data.table::data.table()`. Each row is one configuration. Contains values in the search space. Can contain additional columns for extra information.

`y` (numeric(1))
 Optimal outcome.
`learner_param_vals` (List of named list(s))
 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

```

# Hyperparameter optimization on the Palmer Penguins data set
task = tsk("penguins")

# Load learner and set search space
learner = lrn("classif.rpart",
  cp = to_tune(1e-04, 1e-1, logscale = TRUE)
)

# Construct tuning instance
instance = ti(
  task = task,
  learner = learner,
  resampling = rsmpl("cv", folds = 3),
  measures = msr("classif.ce"),
  terminator = trm("evals", n_evals = 4)
)

# Choose optimization algorithm
tuner = tnr("random_search", batch_size = 2)

# Run tuning
tuner$optimize(instance)

# Set optimal hyperparameter configuration to learner
learner$param_set$values = instance$result_learner_param_vals

# Train the learner on the full data set
learner$train(task)

# Inspect all evaluated configurations
as.data.table(instance$archive)

```

Index

- * **Dictionary**
 - mlr_tuners, 27
- * **Tuner**
 - mlr_tuners, 27
 - mlr_tuners_cmaes, 28
 - mlr_tuners_design_points, 30
 - mlr_tuners_gensa, 32
 - mlr_tuners_grid_search, 35
 - mlr_tuners_irace, 37
 - mlr_tuners_nloptr, 40
 - mlr_tuners_random_search, 43
- * **datasets**
 - mlr_tuners, 27

- adagio::pureCMAES(), 28
- Archive, 60, 64
- ArchiveTuning, 3, 3, 4, 9, 26, 38, 39, 46, 47, 51, 53, 57, 61, 65
- as_search_space, 7
- auto_tuner, 13
- auto_tuner(), 7, 13
- AutoTuner, 7, 7, 8, 13, 15, 16, 21, 23, 25

- bbotk::Archive, 4
- bbotk::CallbackOptimization, 16
- bbotk::Codomain, 5
- bbotk::ContextOptimization, 17–20
- bbotk::Objective, 45
- bbotk::OptimInstance, 61, 65
- bbotk::OptimInstanceMultiCrit, 61
- bbotk::OptimInstanceSingleCrit, 65
- bbotk::OptimizerCmaes, 28
- bbotk::OptimizerDesignPoints, 30
- bbotk::OptimizerGenSA, 33
- bbotk::OptimizerGridSearch, 36
- bbotk::OptimizerIrace, 38
- bbotk::OptimizerNloptr, 41
- bbotk::OptimizerRandomSearch, 43
- bbotk::Terminator, 7, 15, 40, 55, 60, 64

- callback_tuning, 17
- callback_tuning(), 16, 19
- CallbackTuning, 10, 14, 16, 16, 17, 19, 24–26, 46–48, 52, 59, 62, 66
- clbk(), 16, 17
- ContextEval, 17–19, 19
- ContextOptimization, 19

- data.table::data.table, 9, 20, 31, 39
- data.table::data.table(), 3, 4, 21, 23, 27, 57
- dictionary, 16, 17, 50

- extract_inner_tuning_archives, 21
- extract_inner_tuning_results, 22

- GenSA::GenSA(), 32, 33

- irace::defaultScenario(), 38
- irace::irace(), 37

- Learner, 11

- Measures, 53
- mlr3::benchmark(), 8, 15, 16, 21, 23, 30, 33, 36, 43, 55, 60, 64
- mlr3::BenchmarkResult, 3–5, 10, 14, 20–24, 26, 46, 48, 52, 59, 62, 66
- mlr3::HotstartStack, 10, 14, 35, 46–48, 52, 59, 62, 66
- mlr3::Learner, 5, 7–10, 13, 15, 45, 46, 48, 51, 53, 58, 62, 66
- mlr3::Measure, 4, 5, 7, 10, 14, 15, 45, 46, 48, 52, 53, 59, 62, 66
- mlr3::Prediction, 6
- mlr3::resample(), 8, 15, 21, 23
- mlr3::ResampleResult, 4, 6, 21–23, 53, 59, 61, 65
- mlr3::Resampling, 7, 8, 10, 13, 15, 16, 45, 46, 48, 52, 53, 58, 62, 66
- mlr3::Task, 45, 46, 48, 51, 53, 58, 61, 65

- mlr3misc::Callback, [16](#)
- mlr3misc::Context, [20](#)
- mlr3misc::Dictionary, [27](#), [50](#)
- mlr3misc::dictionary_sugar_get(), [50](#)
- mlr3tuning (mlr3tuning-package), [3](#)
- mlr3tuning-package, [3](#)
- mlr3tuning.backup, [24](#)
- mlr3tuning.early_stopping, [25](#)
- mlr3tuning.measures, [26](#)
- mlr3tuning::Tuner, [29](#), [31](#), [34](#), [36](#), [39](#), [41](#), [44](#)
- mlr3tuning::TunerFromOptimizer, [29](#), [31](#), [34](#), [39](#), [41](#), [44](#)
- mlr_callbacks, [16](#), [17](#)
- mlr_reflections\$tuner_properties, [56](#), [57](#)
- mlr_terminators, [50](#)
- mlr_tuners, [27](#), [29](#), [31](#), [34](#), [37](#), [39](#), [42](#), [44](#), [50](#)
- mlr_tuners_cmaes, [27](#), [28](#), [31](#), [34](#), [37](#), [39](#), [42](#), [44](#)
- mlr_tuners_design_points, [27](#), [29](#), [30](#), [34](#), [37](#), [39](#), [42](#), [44](#)
- mlr_tuners_gensa, [27](#), [29](#), [31](#), [32](#), [37](#), [39](#), [42](#), [44](#)
- mlr_tuners_grid_search, [27](#), [29](#), [31](#), [34](#), [35](#), [39](#), [42](#), [44](#)
- mlr_tuners_irace, [27](#), [29](#), [31](#), [34](#), [37](#), [37](#), [42](#), [44](#)
- mlr_tuners_nloptr, [27](#), [29](#), [31](#), [34](#), [37](#), [39](#), [40](#), [44](#)
- mlr_tuners_random_search, [27](#), [29](#), [31](#), [34](#), [37](#), [39](#), [42](#), [43](#)
- nloptr::nloptr, [40](#)
- nloptr::nloptr(), [40](#), [41](#)
- nloptr::nloptr.print.options(), [41](#)
- ObjectiveTuning, [20](#), [45](#), [60](#), [64](#)
- paradox::generate_design_grid(), [35](#)
- paradox::generate_design_random(), [43](#)
- paradox::Param, [56](#), [57](#)
- paradox::ParamSet, [5](#), [7](#), [10](#), [14](#), [15](#), [48](#), [50](#), [52](#), [56](#), [59](#), [62](#), [66](#)
- paradox::TuneToken, [53](#)
- R6, [5](#), [9](#), [20](#), [29](#), [31](#), [34](#), [36](#), [39](#), [42](#), [44](#), [46](#), [56](#), [61](#), [65](#)
- R6::R6Class, [27](#), [50](#)
- requireNamespace(), [56](#), [57](#)
- Terminator, [10](#), [14](#), [28](#), [31](#), [34](#), [36](#), [38](#), [41](#), [44](#), [48](#), [50](#), [52](#), [53](#), [59](#), [62](#), [66](#)
- TerminatorCombo, [53](#)
- TerminatorEvals, [38](#)
- Terminators, [50](#), [53](#)
- ti, [47](#)
- ti(), [60](#), [63](#)
- tnr, [50](#)
- tnr(), [27](#), [28](#), [30](#), [33](#), [35](#), [37](#), [40](#), [43](#)
- tnrs (tnr), [50](#)
- tnrs(), [27](#)
- tune, [51](#)
- tune(), [60](#), [63](#)
- tune_nested, [58](#)
- Tuner, [7](#), [8](#), [10](#), [13–15](#), [27](#), [28](#), [30](#), [33](#), [35–38](#), [40](#), [41](#), [43](#), [46](#), [48](#), [50–52](#), [54](#), [54](#), [58](#), [60](#), [62](#), [64](#), [66](#)
- TunerCmaes (mlr_tuners_cmaes), [28](#)
- TunerDesignPoints (mlr_tuners_design_points), [30](#)
- TunerGenSA (mlr_tuners_gensa), [32](#)
- TunerGridSearch (mlr_tuners_grid_search), [35](#)
- TunerIrace (mlr_tuners_irace), [37](#)
- TunerNloptr (mlr_tuners_nloptr), [40](#)
- TunerRandomSearch (mlr_tuners_random_search), [43](#)
- Tuners, [50](#), [60](#), [63](#)
- TuneToken, [5](#), [10](#), [14](#), [48](#), [52](#), [59](#), [62](#), [66](#)
- TuningInstanceMultiCrit, [23](#), [45](#), [47](#), [48](#), [51–53](#), [55](#), [57](#), [60](#), [60](#)
- TuningInstanceSingleCrit, [8–10](#), [14](#), [23](#), [39](#), [45](#), [47](#), [48](#), [51–53](#), [55](#), [57](#), [59](#), [63](#), [63](#)