# Package: mlr3tuning (via r-universe)

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Title Hyperparameter Optimization for 'mlr3'

Version 1.0.1

**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.

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URL https://mlr3tuning.mlr-org.com,

https://github.com/mlr-org/mlr3tuning

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

**Depends** mlr3 (>= 0.20.0), paradox (>= 1.0.1), R (>= 3.1.0)

Imports bbotk (>= 1.1.0), checkmate (>= 2.0.0), data.table, lgr, mlr3misc (>= 0.15.1), R6

**Suggests** adagio, future, GenSA, irace, knitr, mlflow, mlr3learners (>= 0.7.0), mlr3pipelines (>= 0.5.2), nloptr, rush, rmarkdown, rpart, testthat (>= 3.0.0), xgboost

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Collate 'ArchiveAsyncTuning.R' 'ArchiveBatchTuning.R' 'AutoTuner.R' 'CallbackAsyncTuning.R' 'CallbackBatchTuning.R' 'ContextAsyncTuning.R' 'ContextBatchTuning.R' 'ObjectiveTuning.R' 'ObjectiveTuningAsync.R' 'ObjectiveTuningBatch.R' 'mlr\_tuners.R' 'Tuner.R' 'TunerAsync.R' 'TunerAsyncDesignPoints.R' 'TunerAsyncFromOptimizerAsync.R' 'TunerAsyncGridSearch.R' 'TunerAsyncRandomSearch.R' 'TunerBatch.R' 'TunerBatchCmaes.R' 'TunerBatchDesignPoints.R' 'TunerBatchFromBatchOptimizer.R' 'TunerBatchGenSA.R' 'TunerBatchGridSearch.R' 'TunerBatchInternal.R' 'TunerBatchIrace.R' 'TunerBatchNLoptr.R' 'TunerBatchRandomSearch.R' 'TuningInstanceBatchSingleCrit.R' 'TuningInstanceAsyncMulticrit.R' 'TuningInstanceAsyncSingleCrit.R' 'TuningInstanceBatchMulticrit.R' 'TuningInstanceMultiCrit.R' 'TuningInstanceSingleCrit.R' 'as\_search\_space.R' 'as\_tuner.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'

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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.

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# 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

ArchiveAsyncTuning Rush Data Storage

#### Description

The 'ArchiveAsyncTuning" stores all evaluated hyperparameter configurations and performance scores in a rush::Rush database.

## Details

The ArchiveAsyncTuning is a connector to a rush::Rush database.

# **Data Structure**

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

- One column for each hyperparameter of the search space (\$search\_space).
- One (list-)column for the internal\_tuned\_values
- 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.

## Analysis

For analyzing the tuning results, it is recommended to pass the ArchiveAsyncTuning to as.data.table(). The returned data table contains the mlr3::ResampleResult for each hyperparameter evaluation.

#### S3 Methods

as.data.table.ArchiveTuning(x, unnest = "x\_domain", exclude\_columns = "uhash", measures = NULL)
 Returns a tabular view of all evaluated hyperparameter configurations.

ArchiveAsyncTuning -> data.table::data.table()

- x (ArchiveAsyncTuning)
- 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 classes

bbotk::Archive -> bbotk::ArchiveAsync -> ArchiveAsyncTuning

## Active bindings

internal\_search\_space (paradox::ParamSet) The search space containing those parameters that are internally optimized by the mlr3::Learner.

benchmark\_result (mlr3::BenchmarkResult) Benchmark result.

# Methods

#### **Public methods:**

- ArchiveAsyncTuning\$new()
- ArchiveAsyncTuning\$learner()
- ArchiveAsyncTuning\$learners()
- ArchiveAsyncTuning\$learner\_param\_vals()
- ArchiveAsyncTuning\$predictions()
- ArchiveAsyncTuning\$resample\_result()
- ArchiveAsyncTuning\$print()
- ArchiveAsyncTuning\$clone()

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

Usage:

```
ArchiveAsyncTuning$new(
   search_space,
   codomain,
   rush,
   internal_search_space = NULL
)
```

Arguments:

search\_space (paradox::ParamSet)

Hyperparameter search space. If NULL (default), the search space is constructed from the paradox::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.

```
rush (Rush)
```

If a rush instance is supplied, the tuning runs without batches.

internal\_search\_space (paradox::ParamSet or NULL)

The internal search space of the tuner. This includes parameters that the learner can optimize internally durign *\$train()*, such as the number of epochs via early stopping.

```
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:
ArchiveAsyncTuning$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:
```

ArchiveAsyncTuning\$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:

# ArchiveAsyncTuning

```
ArchiveAsyncTuning$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:
ArchiveAsyncTuning$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:

```
ArchiveAsyncTuning$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:

ArchiveAsyncTuning\$print()

Arguments:

... (ignored).

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

Usage:

ArchiveAsyncTuning\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

ArchiveBatchTuning

#### Description

The ArchiveBatchTuning stores all evaluated hyperparameter configurations and performance scores in a data.table::data.table().

## Details

The ArchiveBatchTuning 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 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 (list-)column for the internal\_tuned\_values
- 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 ArchiveBatchTuning 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.

#### ArchiveBatchTuning

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. ArchiveBatchTuning -> data.table::data.table()

- x (ArchiveBatchTuning)
- 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 classes

bbotk::Archive -> bbotk::ArchiveBatch -> ArchiveBatchTuning

#### **Public fields**

benchmark\_result (mlr3::BenchmarkResult) Benchmark result.

## Active bindings

internal\_search\_space (paradox::ParamSet) The search space containing those parameters that are internally optimized by the mlr3::Learner.

# Methods

#### **Public methods:**

- ArchiveBatchTuning\$new()
- ArchiveBatchTuning\$learner()
- ArchiveBatchTuning\$learners()
- ArchiveBatchTuning\$learner\_param\_vals()
- ArchiveBatchTuning\$predictions()
- ArchiveBatchTuning\$resample\_result()
- ArchiveBatchTuning\$print()
- ArchiveBatchTuning\$clone()

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

Usage:

```
ArchiveBatchTuning$new(
   search_space,
   codomain,
   check_values = FALSE,
   internal_search_space = NULL
)
```

Arguments:

search\_space (paradox::ParamSet)

Hyperparameter search space. If NULL (default), the search space is constructed from the paradox::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.

internal\_search\_space (paradox::ParamSet or NULL)

The internal search space of the tuner. This includes parameters that the learner can optimize internally durign *train()*, such as the number of epochs via early stopping.

**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:
ArchiveBatchTuning$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:

ArchiveBatchTuning\$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:

ArchiveBatchTuning\$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:
ArchiveBatchTuning$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:

```
ArchiveBatchTuning$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:

ArchiveBatchTuning\$print()

Arguments:

... (ignored).

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

#### Usage:

ArchiveBatchTuning\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

as\_search\_space

# 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

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

## Value

paradox::ParamSet.

as\_tuner

Convert to a Tuner

# Description

Convert object to a Tuner or a list of Tuner.

# Usage

```
as_tuner(x, ...)
## S3 method for class 'Tuner'
as_tuner(x, clone = FALSE, ...)
as_tuners(x, ...)
## Default S3 method:
```

# AutoTuner

```
as_tuners(x, ...)
## S3 method for class 'list'
as_tuners(x, ...)
```

#### Arguments

x	(any) Object to convert.
	(any) Additional arguments.
clone	(logical(1)) Whether to clone the object.

AutoTuner

#### Class 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.

#### **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.

# Validation

The AutoTuner itself does **not** have the "validation" property. To enable validation during the tuning, set the \$validate field of the tuned learner. This is also possible via set\_validate().

#### 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 TuningInstanceBatchSingleCrit.

tuner (Tuner)

Optimization algorithm.

# Active bindings

internal\_valid\_scores Retrieves the inner validation scores as a named list(). Returns NULL if learner is not trained yet.

archive ArchiveBatchTuning

Archive of the TuningInstanceBatchSingleCrit.

# AutoTuner

learner (mlr3::Learner)

Trained learner

tuning\_instance (TuningInstanceAsyncSingleCrit | TuningInstanceBatchSingleCrit) Internally created tuning instance with all intermediate results.

tuning\_result (data.table::data.table)

Short-cut to result from tuning instance.

```
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\$oob\_error()
- AutoTuner\$loglik()
- AutoTuner\$print()
- AutoTuner\$marshal()
- AutoTuner\$unmarshal()
- AutoTuner\$marshaled()
- 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,
   callbacks = NULL,
   rush = NULL
)
```

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 (bbotk::Terminator)

Stop criterion of the tuning process.

#### search\_space (paradox::ParamSet)

Hyperparameter search space. If NULL (default), the search space is constructed from the paradox::TuneToken of the learner's parameter set (learner\$param\_set).

#### store\_tuning\_instance (logical(1))

If TRUE (default), stores the internally created TuningInstanceBatchSingleCrit 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.

## callbacks (list of mlr3misc::Callback)

- List of callbacks.
- rush (Rush)

If a rush instance is supplied, the tuning runs without batches.

**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: mlr3::Learner.

# AutoTuner

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 marshal(): Marshal the learner.

Usage:

AutoTuner\$marshal(...)

Arguments:

... (any) Additional parameters.

Returns: self

# Method unmarshal(): Unmarshal the learner.

Usage: AutoTuner\$unmarshal(...)

Arguments:

... (any) Additional parameters.

Returns: self

Method marshaled(): Whether the learner is marshaled.

Usage: AutoTuner\$marshaled()

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

auto\_tuner

```
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,
  callbacks = NULL,
  rush = NULL
)
```

# 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 con- figurations. 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	(bbotk::Terminator) Stop criterion of the tuning process.
search_space	(paradox::ParamSet) Hyperparameter search space. If NULL (default), the search space is constructed from the paradox::TuneToken of the learner's parameter set (learner\$param_set).
store_tuning_ir	nstance
	(logical(1)) If TRUE (default), stores the internally created TuningInstanceBatchSingleCrit with all intermediate results in slot \$tuning_instance.
store_benchmark	<_result
	(logical(1)) If TRUE (default), store resample result of evaluated hyperparameter configura- tions in archive as mlr3::BenchmarkResult.
store_models	<pre>(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.</pre>
check_values	(logical(1)) If TRUE, hyperparameter values are checked before evaluation and performance scores after. If FALSE (default), values are unchecked but computational over- head is reduced.
callbacks	(list of mlr3misc::Callback) List of callbacks.
rush	(Rush) If a rush instance is supplied, the tuning runs without batches.

#### auto\_tuner

#### 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"))
```

CallbackAsyncTuning Create Asynchronous Tuning Callback

#### Description

Specialized bbotk::CallbackAsync for asynchronous tuning. Callbacks allow to customize the behavior of processes in mlr3tuning. The callback\_async\_tuning() function creates a Callback-AsyncTuning. Predefined callbacks are stored in the dictionary mlr\_callbacks and can be retrieved with clbk(). For more information on tuning callbacks see callback\_async\_tuning().

#### Super classes

mlr3misc::Callback -> bbotk::CallbackAsync -> CallbackAsyncTuning

#### **Public fields**

```
on_eval_after_xs (function())
    Stage called after xs is passed. Called in ObjectiveTuning$eval().
```

on\_eval\_after\_resample (function())
Stage called after hyperparameter configurations are evaluated. Called in ObjectiveTuning\$eval().

on\_eval\_before\_archive (function()) Stage called before performance values are written to the archive. Called in ObjectiveTuning\$eval().

#### Methods

# **Public methods:**

CallbackAsyncTuning\$clone()

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

Usage:

CallbackAsyncTuning\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

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## Description

Specialized bbotk::CallbackBatch for batch tuning. Callbacks allow to customize the behavior of processes in mlr3tuning. The callback\_batch\_tuning() function creates a CallbackBatchTuning. Predefined callbacks are stored in the dictionary mlr\_callbacks and can be retrieved with clbk(). For more information on tuning callbacks see callback\_batch\_tuning().

#### Super classes

mlr3misc::Callback -> bbotk::CallbackBatch -> CallbackBatchTuning

# **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:**

CallbackBatchTuning\$clone()

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

Usage:

CallbackBatchTuning\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

## Examples

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

callback\_async\_tuning Create Asynchronous Tuning Callback

#### Description

Function to create a CallbackAsyncTuning. Predefined callbacks are stored in the dictionary mlr\_callbacks and can be retrieved with clbk().

Tuning callbacks can be called from different stages of the tuning process. The stages are prefixed with on\_\*.

```
Start Tuning
     - on_optimization_begin
    Start Worker
         - on_worker_begin
         Start Optimization on Worker
           - on_optimizer_before_eval
             Start Evaluation
               - on_eval_after_xs
               - on_eval_after_resample
               - on_eval_before_archive
             End Evaluation
          - on_optimizer_after_eval
         End Optimization on Worker
         - on_worker_end
    End Worker
     - on_result
     - on_optimization_end
End Tuning
```

See also the section on parameters for more information on the stages. A tuning callback works with ContextAsyncTuning.

#### Usage

```
callback_async_tuning(
    id,
    label = NA_character_,
    man = NA_character_,
    on_optimization_begin = NULL,
    on_worker_begin = NULL,
    on_optimizer_before_eval = NULL,
    on_eval_after_resample = NULL,
    on_eval_before_archive = NULL,
    on_optimizer_after_eval = NULL,
    on_worker_end = 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().
on_worker_begir	
	(function()) Stage called at the beginning of the optimization on the worker. Called in the worker loop.
on_optimizer_be	fore_eval
	(function()) Stage called after the optimizer proposes points. Called in OptimInstance\$.eval_point().
on_eval_after_x	S
	(function()) Stage called after xs is passed. Called in ObjectiveTuning\$eval().
on_eval_after_r	resample
	(function()) Stage called after a hyperparameter configuration is evaluated. Called in ObjectiveTuning\$eval().
on_eval_before_	archive
	<pre>(function()) Stage called before performance values are written to the archive. Called in ObjectiveTuning\$eval().</pre>
on_optimizer_af	`ter_eval
	(function()) Stage called after points are evaluated. Called in OptimInstance\$.eval_point().
on_worker_end	(function()) Stage called at the end of the optimization on the worker. Called in the worker loop.
on_result	(function()) Stage called after the result is written. Called in OptimInstance\$assign_result().
on_optimization	_end
	(function()) Stage called at the end of the optimization. Called in Optimizer\$optimize().

## Details

When implementing a callback, each function 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. Tuning callbacks access ContextAsyncTuning.

callback\_batch\_tuning Create Batch Tuning Callback

## Description

Function to create a CallbackBatchTuning. Predefined callbacks are stored in the dictionary mlr\_callbacks and can be retrieved with clbk().

Tuning callbacks can be called from different stages of the tuning process. The stages are prefixed with on\_\*.

#### Start Tuning

See also the section on parameters for more information on the stages. A tuning callback works with ContextBatchTuning.

## Usage

```
callback_batch_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	<pre>(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().</pre>
on_optimization	_begin
	(function()) Stage called at the beginning of the optimization. Called in Optimizer\$optimize().
on_optimizer_be	fore_eval
	(function()) Stage called after the optimizer proposes points. Called in OptimInstance\$eval_batch().
on_eval_after_d	esign
	<pre>(function()) Stage called after the design is created. Called in ObjectiveTuning\$eval_many(). The context available is ContextBatchTuning.</pre>
on_eval_after_b	enchmark
	<pre>(function()) Stage called after hyperparameter configurations are evaluated. Called in ObjectiveTuning\$eval_many( The context available is ContextBatchTuning.</pre>
on_eval_before_	archive
	<pre>(function()) Stage called before performance values are written to the archive. Called in ObjectiveTuning\$eval_many(). The context available is ContextBatchTun- ing.</pre>
on_optimizer_af	ter_eval
	(function()) Stage called after points are evaluated. Called in OptimInstance\$eval_batch().
on_result	(function()) Stage called after the result is written. Called in OptimInstance\$assign_result().
on_optimization	_end
	(function()) Stage called at the end of the optimization. Called in Optimizer\$optimize().

# Details

When implementing a callback, each function 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. Tuning callbacks access ContextBatchTuning.

# Examples

```
# write archive to disk
callback_batch_tuning("mlr3tuning.backup",
```

```
on_optimization_end = function(callback, context) {
   saveRDS(context$instance$archive, "archive.rds")
}
```

ContextAsyncTuning Asynchronous Tuning Context

## Description

A CallbackAsyncTuning accesses and modifies data during the optimization via the ContextAsyncTuning. See the section on active bindings for a list of modifiable objects. See callback\_async\_tuning() for a list of stages that access ContextAsyncTuning.

# Details

Changes to \$instance and \$optimizer in the stages executed on the workers are not reflected in the main process.

#### Super classes

mlr3misc::Context -> bbotk::ContextAsync -> ContextAsyncTuning

# Active bindings

```
hpc_xs (list())
```

The hyperparameter configuration currently evaluated. Contains the values on the learner scale i.e. transformations are applied.

```
resample_result (mlr3::BenchmarkResult)
```

The resample result of the hyperparameter configuration currently evaluated.

```
aggregated_performance (list())
```

Aggregated performance scores and training time of the evaluated hyperparameter configuration. This list is passed to the archive. A callback can add additional elements which are also written to the archive.

# Methods

#### **Public methods:**

ContextAsyncTuning\$clone()

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

Usage:

ContextAsyncTuning\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

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# Description

A CallbackBatchTuning accesses and modifies data during the optimization via the ContextBatchTuning. See the section on active bindings for a list of modifiable objects. See callback\_batch\_tuning() for a list of stages that access ContextBatchTuning.

#### Super classes

mlr3misc::Context -> bbotk::ContextBatch -> ContextBatchTuning

## 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 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:**

ContextBatchTuning\$clone()

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

Usage:

ContextBatchTuning\$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

Х	(mlr3::ResampleResult   mlr3::BenchmarkResult).
unnest	(character())
	Transforms list columns to separate columns. By default, x_domain is unnested.
	Set to NULL if no column should be unnested.
exclude_columns	
	(character())
	Exclude columns from result table. Set to NULL 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 = rsmp ("holdout"),
  measure = msr("classif.ce"),
  term_evals = 4)
resampling_outer = rsmp("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

х	(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 (TuningInstanceBatchSingleCrit | TuningInstanceBatchMultiCrit) 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 = rsmp ("holdout"),
  measure = msr("classif.ce"),
  term_evals = 4)
resampling_outer = rsmp("cv", folds = 2)
rr = resample(tsk("iris"), at, resampling_outer, store_models = TRUE)
# extract inner results
extract_inner_tuning_results(rr)
```

mlr3tuning.asnyc\_mlflow

MLflow Connector Callback

# Description

This mlr3misc::Callback logs the hyperparameter configurations and the performance of the configurations to MLflow.

# Examples

```
clbk("mlr3tuning.async_mlflow", tracking_uri = "http://localhost:5000")
## Not run:
rush::rush_plan(n_workers = 4)
learner = lrn("classif.rpart",
    minsplit = to_tune(2, 128),
    cp = to_tune(1e-04, 1e-1))
instance = TuningInstanceAsyncSingleCrit$new(
    task = tsk("pima"),
    learner = learner,
    resampling = rsmp("cv", folds = 3),
```

```
measure = msr("classif.ce"),
terminator = trm("evals", n_evals = 20),
store_benchmark_result = FALSE,
callbacks = clbk("mlr3tuning.rush_mlflow", tracking_uri = "http://localhost:8080")
)
tuner = tnr("random_search_v2")
tuner$optimize(instance)
## End(Not run)
```

# Description

These CallbackAsyncTuning and CallbackBatchTuning evaluate the default hyperparameter values of a learner.

# Description

This CallbackAsyncTuning saves the logs of the learners to the archive.

mlr3tuning.backup Backup Benchmark Result Callback

# Description

This mlr3misc::Callback writes the mlr3::BenchmarkResult after each batch to disk.

#### mlr3tuning.measures

## 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 = rsmp("cv", folds = 3),
  measures = msr("classif.ce"),
  term_evals = 4,
  callbacks = clbk("mlr3tuning.backup", path = tempfile(fileext = ".rds"))
)
```

mlr3tuning.measures Measure Callback

# Description

This mlr3misc::Callback scores the hyperparameter configurations on additional measures while tuning. Usually, the configurations can be scored on additional measures after tuning (see Archive-BatchTuning). 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"))
)
```

mlr\_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: Tuner, mlr\_tuners\_cmaes, mlr\_tuners\_design\_points, mlr\_tuners\_gensa, mlr\_tuners\_grid\_search, mlr\_tuners\_internal, 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\_async\_design\_points

Hyperparameter Tuning with Asynchronous Design Points

## Description

Subclass for asynchronous design points tuning.

#### Dictionary

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

```
tnr("async_design_points")
```

#### Parameters

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

# Super classes

mlr3tuning::Tuner.>mlr3tuning::TunerAsync.>mlr3tuning::TunerAsyncFromOptimizerAsync ->TunerAsyncDesignPoints

# Methods

#### **Public methods:**

- TunerAsyncDesignPoints\$new()
- TunerAsyncDesignPoints\$clone()

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

Usage:

TunerAsyncDesignPoints\$new()

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

Usage:

TunerAsyncDesignPoints\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

#### See Also

Other TunerAsync: mlr\_tuners\_async\_grid\_search, mlr\_tuners\_async\_random\_search

mlr\_tuners\_async\_grid\_search

Hyperparameter Tuning with Asynchronous Grid Search

# Description

Subclass for asynchronous grid search tuning.

#### Dictionary

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

```
tnr("async_design_points")
```

#### **Parameters**

batch\_size integer(1) Maximum number of points to try in a batch.

# Super classes

mlr3tuning::Tuner.>mlr3tuning::TunerAsync.>mlr3tuning::TunerAsyncFromOptimizerAsync
->TunerAsyncGridSearch

# Methods

#### **Public methods:**

- TunerAsyncGridSearch\$new()
- TunerAsyncGridSearch\$clone()

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

Usage:

TunerAsyncGridSearch\$new()

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

Usage:

TunerAsyncGridSearch\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

# See Also

Other TunerAsync: mlr\_tuners\_async\_design\_points, mlr\_tuners\_async\_random\_search

mlr\_tuners\_async\_random\_search

Hyperparameter Tuning with Asynchronous Random Search

# Description

Subclass for asynchronous 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("async_random_search")
```

## Super classes

```
mlr3tuning::Tuner.>mlr3tuning::TunerAsync.>mlr3tuning::TunerAsyncFromOptimizerAsync
->TunerAsyncRandomSearch
```

#### Methods

#### **Public methods:**

- TunerAsyncRandomSearch\$new()
- TunerAsyncRandomSearch\$clone()

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

Usage:

TunerAsyncRandomSearch\$new()

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

Usage:

TunerAsyncRandomSearch\$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

Other TunerAsync: mlr\_tuners\_async\_design\_points, mlr\_tuners\_async\_grid\_search

mlr\_tuners\_cmaes

#### 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 bbotk::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::OptimizerBatchCmaes 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.

- An overview of all tuners can be found on our website.
- Learn more about tuners.

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

• Use the Hyperband optimizer with different budget parameters.

#### mlr\_tuners\_cmaes

#### Super classes

mlr3tuning::Tuner -> mlr3tuning::TunerBatch -> mlr3tuning::TunerBatchFromOptimizerBatch
-> TunerBatchCmaes

## Methods

# **Public methods:**

- TunerBatchCmaes\$new()
- TunerBatchCmaes\$clone()

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

Usage: TunerBatchCmaes\$new()

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

Usage:

TunerBatchCmaes\$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: Tuner, mlr\_tuners, mlr\_tuners\_design\_points, mlr\_tuners\_gensa, mlr\_tuners\_grid\_search, mlr\_tuners\_internal, mlr\_tuners\_irace, mlr\_tuners\_nloptr, mlr\_tuners\_random\_search

# 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 = 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\_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 batchfashion 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::OptimizerBatchDesignPoints 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.

- An overview of all tuners can be found on our website.
- 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::TunerBatch -> mlr3tuning::TunerBatchFromOptimizerBatch
-> TunerBatchDesignPoints

## Methods

#### **Public methods:**

- TunerBatchDesignPoints\$new()
- TunerBatchDesignPoints\$clone()

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

Usage: TunerBatchDesignPoints\$new()

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

Usage:

TunerBatchDesignPoints\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

#### See Also

Package mlr3hyperband for hyperband tuning.

Other Tuner: Tuner, mlr\_tuners, mlr\_tuners\_cmaes, mlr\_tuners\_gensa, mlr\_tuners\_grid\_search, mlr\_tuners\_internal, mlr\_tuners\_irace, mlr\_tuners\_nloptr, mlr\_tuners\_random\_search

# 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,
                    64,
  0.1, 2,
  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 = rsmp("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::OptimizerBatchGenSA 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.

- An overview of all tuners can be found on our website.
- 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::TunerBatch -> mlr3tuning::TunerBatchFromOptimizerBatch
-> TunerBatchGenSA

#### Methods

#### **Public methods:**

- TunerBatchGenSA\$new()
- TunerBatchGenSA\$clone()

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

Usage: TunerBatchGenSA\$new()

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

Usage:

TunerBatchGenSA\$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: Tuner, mlr\_tuners, mlr\_tuners\_cmaes, mlr\_tuners\_design\_points, mlr\_tuners\_grid\_search, mlr\_tuners\_internal, mlr\_tuners\_irace, mlr\_tuners\_nloptr, mlr\_tuners\_random\_search

## 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 bbotk::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 batchfashion 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::OptimizerBatchGridSearch 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.

- An overview of all tuners can be found on our website.
- 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::TunerBatch -> mlr3tuning::TunerBatchFromOptimizerBatch
-> TunerBatchGridSearch

# Methods

#### **Public methods:**

- TunerBatchGridSearch\$new()
- TunerBatchGridSearch\$clone()

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

Usage:

#### mlr\_tuners\_internal

TunerBatchGridSearch\$new()

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

Usage:

TunerBatchGridSearch\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

## See Also

Other Tuner: Tuner, mlr\_tuners, mlr\_tuners\_cmaes, mlr\_tuners\_design\_points, mlr\_tuners\_gensa, mlr\_tuners\_internal, mlr\_tuners\_irace, mlr\_tuners\_nloptr, mlr\_tuners\_random\_search

# 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 = 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\_internal Hyperparameter Tuning with Internal Tuning

# Description

Subclass to conduct only internal hyperparameter tuning for a mlr3::Learner.

## Dictionary

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

tnr("internal")

# **Progress Bars**

\$optimize() supports progress bars via the package progressr combined with a bbotk::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.

# Resources

There are several sections about hyperparameter optimization in the mlr3book.

- An overview of all tuners can be found on our website.
- 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::TunerBatch -> TunerBatchInternal

# Methods

#### **Public methods:**

- TunerBatchInternal\$new()
- TunerBatchInternal\$clone()

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

Usage: TunerBatchInternal\$new()

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

Usage: TunerBatchInternal\$clone(deep = FALSE)
Arguments:

deep Whether to make a deep clone.

#### mlr\_tuners\_irace

#### Note

The selected mlr3::Measure does not influence the tuning result. To change the loss-function for the internal tuning, consult the hyperparameter documentation of the tuned mlr3::Learner.

# See Also

Other Tuner: Tuner, mlr\_tuners, 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

```
library(mlr3learners)
# Retrieve task
task = tsk("pima")
# Load learner and set search space
learner = lrn("classif.xgboost",
  nrounds = to_tune(upper = 1000, internal = TRUE),
  early_stopping_rounds = 10,
  validate = "test",
  eval_metric = "merror"
)
# Internal hyperparameter tuning on the pima indians diabetes data set
instance = tune(
  tnr("internal"),
  tsk("iris"),
  learner,
  rsmp("cv", folds = 3),
  msr("internal_valid_score", minimize = TRUE, select = "merror")
)
# best performing hyperparameter configuration
instance$result_learner_param_vals
instance$result_learner_param_vals$internal_tuned_values
```

#### Description

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

Hyperparameter Tuning with Iterated Racing.

# Dictionary

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

tnr("irace")

mlr\_tuners\_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 bbotk::TerminatorEvals instead. Other terminators do not work with TunerIrace.

# Archive

The ArchiveBatchTuning 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 bbotk::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::OptimizerBatchIrace 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.

- An overview of all tuners can be found on our website.
- Learn more about tuners.

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

• Use the Hyperband optimizer with different budget parameters.

#### mlr\_tuners\_irace

#### Super classes

mlr3tuning::Tuner -> mlr3tuning::TunerBatch -> mlr3tuning::TunerBatchFromOptimizerBatch
-> TunerBatchIrace

# Methods

#### **Public methods:**

- TunerBatchIrace\$new()
- TunerBatchIrace\$optimize()
- TunerBatchIrace\$clone()

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

Usage: TunerBatchIrace\$new()

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

Usage: TunerBatchIrace\$optimize(inst)
Arguments:

inst (TuningInstanceBatchSingleCrit).

*Returns:* data.table::data.table.

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

Usage:

```
TunerBatchIrace$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.

## See Also

Other Tuner: Tuner, mlr\_tuners, mlr\_tuners\_cmaes, mlr\_tuners\_design\_points, mlr\_tuners\_gensa, mlr\_tuners\_grid\_search, mlr\_tuners\_internal, mlr\_tuners\_nloptr, mlr\_tuners\_random\_search

## 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 = rsmp("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::OptimizerBatchNLoptr 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.

- An overview of all tuners can be found on our website.
- 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::TunerBatch -> mlr3tuning::TunerBatchFromOptimizerBatch
-> TunerBatchNLoptr

# Methods

#### **Public methods:**

- TunerBatchNLoptr\$new()
- TunerBatchNLoptr\$clone()

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

Usage:

TunerBatchNLoptr\$new()

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

Usage:

TunerBatchNLoptr\$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: Tuner, mlr\_tuners, mlr\_tuners\_cmaes, mlr\_tuners\_design\_points, mlr\_tuners\_gensa, mlr\_tuners\_grid\_search, mlr\_tuners\_internal, mlr\_tuners\_irace, mlr\_tuners\_random\_search

# 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 = rsmp("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 batchfashion 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::OptimizerBatchRandomSearch 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.

- An overview of all tuners can be found on our website.
- 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::TunerBatch -> mlr3tuning::TunerBatchFromOptimizerBatch
-> TunerBatchRandomSearch

# Methods

# **Public methods:**

- TunerBatchRandomSearch\$new()
- TunerBatchRandomSearch\$clone()

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

Usage:

TunerBatchRandomSearch\$new()

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

Usage:

TunerBatchRandomSearch\$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: Tuner, mlr\_tuners, mlr\_tuners\_cmaes, mlr\_tuners\_design\_points, mlr\_tuners\_gensa, mlr\_tuners\_grid\_search, mlr\_tuners\_internal, mlr\_tuners\_irace, mlr\_tuners\_nloptr

# **ObjectiveTuning**

# 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 = 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"))
```

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 TuningInstanceBatchSingleCrit or TuningInstanceBatchMultiCrit.

## 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)).
```

callbacks (List of mlr3misc::Callback).

default\_values (named list()).

internal\_search\_space (paradox::ParamSet). Internal search space for internal tuning.

# 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 = FALSE,
   callbacks = NULL,
   internal_search_space = NULL
)
```

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.

callbacks (list of mlr3misc::Callback)

List of callbacks.

internal\_search\_space (paradox::ParamSet or NULL)

The internal search space of the tuner. This includes parameters that the learner can optimize internally durign \$train(), such as the number of epochs via early stopping.

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.

ObjectiveTuningAsync Class for Tuning Objective

# Description

Stores the objective function that estimates the performance of hyperparameter configurations. This class is usually constructed internally by the TuningInstanceBatchSingleCrit or TuningInstanceBatchMultiCrit.

# Super classes

bbotk::Objective -> mlr3tuning::ObjectiveTuning -> ObjectiveTuningAsync

#### Methods

#### **Public methods:**

ObjectiveTuningAsync\$clone()

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

Usage:

ObjectiveTuningAsync\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

ObjectiveTuningBatch Class for Tuning Objective

#### Description

Stores the objective function that estimates the performance of hyperparameter configurations. This class is usually constructed internally by the TuningInstanceBatchSingleCrit or TuningInstanceBatchMultiCrit.

## Super classes

bbotk::Objective -> mlr3tuning::ObjectiveTuning -> ObjectiveTuningBatch

# **Public fields**

archive (ArchiveBatchTuning).

# Methods

**Public methods:** 

- ObjectiveTuningBatch\$new()
- ObjectiveTuningBatch\$clone()

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

```
Usage:
ObjectiveTuningBatch$new(
  task,
  learner,
  resampling,
  measures,
  store_benchmark_result = TRUE,
  store_models = FALSE,
  check_values = FALSE,
  archive = NULL,
  callbacks = NULL,
  internal_search_space = NULL
)
```

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.

```
archive (ArchiveBatchTuning)
```

Reference to archive of TuningInstanceBatchSingleCrit | TuningInstanceBatchMultiCrit. If NULL (default), benchmark result and models cannot be stored.

# callbacks (list of mlr3misc::Callback)

List of callbacks.

```
internal_search_space (paradox::ParamSet or NULL)
```

The internal search space of the tuner. This includes parameters that the learner can optimize internally durign *\$train()*, such as the number of epochs via early stopping.

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

#### Usage:

ObjectiveTuningBatch\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

set\_validate.AutoTuner

Configure Validation for AutoTuner

## Description

Configure validation data for the learner that is tuned by the AutoTuner.

#### Usage

```
## S3 method for class 'AutoTuner'
set_validate(learner, validate, ...)
```

# Arguments

learner	(AutoTuner) The autotuner for which to enable validation.
validate	(numeric(1), "predefined", "test", or NULL) How to configure the validation during the hyperparameter tuning.
	(any) Passed when calling set_validate() on the wrapped leaerner.

# Examples

```
at = auto_tuner(
  tuner = tnr("random_search"),
  learner = lrn("classif.debug", early_stopping = TRUE,
    iter = to_tune(upper = 1000L, internal = TRUE), validate = 0.2),
  resampling = rsmp("holdout")
)
# use the test set as validation data during tuning
set_validate(at, validate = "test")
at$learner$validate
```

```
Syntactic Sugar for Tuning Instance Construction
```

# Description

ti

Function to construct a TuningInstanceBatchSingleCrit or TuningInstanceBatchMultiCrit.

# Usage

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

# 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 con- figurations. 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 TuningInstanceBatchSingleCrit and multiple mea- sures a TuningInstanceBatchMultiCrit. If NULL, default measure is used.
terminator	(bbotk::Terminator)
	Stop criterion of the tuning process.
search_space	(paradox::ParamSet)
	Hyperparameter search space. If NULL (default), the search space is constructed
	from the paradox::TuneToken of the learner's parameter set (learner\$param_set).
store_benchmar	k_result
	(logical(1)) If TRUE (default), store resample result of evaluated hyperparameter configura- tions in archive as mlr3: Ranchmark Result
atana madala	(logical(1))
store_models	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 over- head is reduced.
callbacks	(list of mlr3misc::Callback) 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.

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 = rsmp("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)
```

ti\_async

# Description

Function to construct a TuningInstanceAsyncSingleCrit or TuningInstanceAsyncMultiCrit.

# Usage

```
ti_async(
   task,
   learner,
   resampling,
   measures = NULL,
   terminator,
   search_space = NULL,
   store_benchmark_result = TRUE,
   store_models = FALSE,
   check_values = FALSE,
   callbacks = NULL,
   rush = NULL
)
```

# 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 con- figurations. 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 TuningInstanceAsyncSingleCrit and multiple mea- sures a TuningInstanceAsyncMultiCrit. If NULL, default measure is used.
terminator	(bbotk::Terminator) Stop criterion of the tuning process.
search_space	(paradox::ParamSet) Hyperparameter search space. If NULL (default), the search space is constructed from the paradox::TuneToken of the learner's parameter set (learner\$param_set).

store_benchmark	_result
	(logical(1)) If TRUE (default), store resample result of evaluated hyperparameter configura- tions in archive as mlr3::BenchmarkResult.
store_models	<pre>(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.</pre>
check_values	(logical(1)) If TRUE, hyperparameter values are checked before evaluation and performance scores after. If FALSE (default), values are unchecked but computational over- head is reduced.
callbacks	(list of mlr3misc::Callback) List of callbacks.
rush	(Rush) If a rush instance is supplied, the tuning runs without batches.

# 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

## tnr

# 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 = rsmp("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 bbotk::Terminator from mlr\_terminators.
- trms() for a list of Terminators from mlr\_terminators.

#### Usage

tnr(.key, ...)

tnrs(.keys, ...)

## Arguments

.key	(character(1))	
	Key passed to the respective dictionary to retrieve the object.	
	(any) Additional arguments.	
.keys	(character()) Keys passed to the respective dictionary 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 TuningInstanceBatchSingleCrit or TuningInstanceBatchMultiCrit which describes the tuning problem. It executes the tuning with the Tuner (tuner) and returns the result with the tuning instance (\$result). The ArchiveBatchTuning and ArchiveAsyncTuning (\$archive) stores all evaluated hyperparameter configurations and performance scores.

You can find an overview of all tuners on our website.

## 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,
callbacks = NULL,
rush = NULL
```

```
)
```

# 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 con- figurations. 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 TuningInstanceBatchSingleCrit and multiple mea- sures a TuningInstanceBatchMultiCrit. 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	(bbotk::Terminator) Stop criterion of the tuning process.
search_space	(paradox::ParamSet) Hyperparameter search space. If NULL (default), the search space is constructed from the paradox::TuneToken of the learner's parameter set (learner\$param_set).
store_benchmar	<pre>k_result   (logical(1))   If TRUE (default), store resample result of evaluated hyperparameter configura-   tions in archive as mlr3::BenchmarkResult.</pre>
store_models	<pre>(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.</pre>

check_values	(logical(1)) If TRUE, hyperparameter values are checked before evaluation and performance scores after. If FALSE (default), values are unchecked but computational over- head is reduced.
callbacks	(list of mlr3misc::Callback) List of callbacks.
rush	(Rush) If a rush instance is supplied, the tuning runs without batches.

### Details

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The mlr3::Task, mlr3::Learner, mlr3::Resampling, mlr3::Measure and bbotk::Terminator are used to construct a TuningInstanceBatchSingleCrit. If multiple performance mlr3::Measures are supplied, a TuningInstanceBatchMultiCrit is created. The parameter term\_evals and term\_time are shortcuts to create a bbotk::Terminator. If both parameters are passed, a bbotk::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

TuningInstanceBatchSingleCrit | TuningInstanceBatchMultiCrit

#### 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"	mlr3spatia
"regr_st"	"regr.mse"	mlr3spatial
Tuner

"clust" "clust.dunn" mlr3cluster

#### Analysis

For analyzing the tuning results, it is recommended to pass the ArchiveBatchTuning 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 = rsmp ("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

Tuner

#### Description

The Tuner implements the optimization algorithm.

## Details

Tuner is an abstract base class that implements the base functionality each tuner must provide.

#### Resources

There are several sections about hyperparameter optimization in the mlr3book.

- An overview of all tuners can be found on our website.
- 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, as given in the paradox::ParamSet \$class field.

```
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().

Tuner

## Methods

#### **Public methods:**

- Tuner\$new()
- Tuner\$format()
- Tuner\$print()
- Tuner\$help()
- 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, as
     given in the paradox::ParamSet $class field.
 properties (character())
     Set of properties of the tuner. Must be a subset of mlr_reflections$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 refer-
     enced 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 clone(): The objects of this class are cloneable with this method.

Usage: Tuner\$clone(deep = FALSE) Arguments:

deep Whether to make a deep clone.

## See Also

```
Other Tuner: mlr_tuners, mlr_tuners_cmaes, mlr_tuners_design_points, mlr_tuners_gensa, mlr_tuners_grid_search, mlr_tuners_internal, mlr_tuners_irace, mlr_tuners_nloptr, mlr_tuners_random_sear
```

TunerAsync

Class for Asynchronous Tuning Algorithms

## Description

The TunerAsync implements the asynchronous optimization algorithm.

## Details

TunerAsync is an abstract base class that implements the base functionality each asynchronous tuner must provide.

## Resources

There are several sections about hyperparameter optimization in the mlr3book.

- An overview of all tuners can be found on our website.
- 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 -> TunerAsync

## **TunerBatch**

#### Methods

#### **Public methods:**

- TunerAsync\$optimize()
- TunerAsync\$clone()

**Method** optimize(): Performs the tuning on a TuningInstanceAsyncSingleCrit or TuningInstanceAsyncMultiCrit until termination. The single evaluations will be written into the ArchiveAsync-Tuning that resides in the TuningInstanceAsyncSingleCrit/TuningInstanceAsyncMultiCrit. The result will be written into the instance object.

Usage:

TunerAsync\$optimize(inst)

Arguments:

inst (TuningInstanceAsyncSingleCrit | TuningInstanceAsyncMultiCrit).

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

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

Usage: TunerAsync\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

TunerBatch

Class for Batch Tuning Algorithms

#### Description

The TunerBatch implements the optimization algorithm.

#### Details

TunerBatch 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 TuningInstanceBatchSingleCrit/TuningInstanceBatchMultiCrit object instance, so each batch is possibly executed in parallel via mlr3::benchmark(), and all evaluations are stored 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.

- An overview of all tuners can be found on our website.
- 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 -> TunerBatch

#### Methods

#### **Public methods:**

- TunerBatch\$new()
- TunerBatch\$optimize()
- TunerBatch\$clone()

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

```
Usage:
TunerBatch$new(
  id = "tuner_batch",
  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, as given in the paradox::ParamSet \$class field.

```
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** optimize(): Performs the tuning on a TuningInstanceBatchSingleCrit or TuningInstanceBatchMultiCrit until termination. The single evaluations will be written into the Archive-BatchTuning that resides in the TuningInstanceBatchSingleCrit/TuningInstanceBatchMultiCrit. The result will be written into the instance object.

Usage:

TunerBatch\$optimize(inst)

Arguments:

inst (TuningInstanceBatchSingleCrit | TuningInstanceBatchMultiCrit).

Returns: data.table::data.table()

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

Usage:

TunerBatch\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

tune\_nested

## 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,
  callbacks = NULL
)
```

## Arguments

tuner	(Tuner) Optimization algorithm.
task	(mlr3::Task) Task to operate on.
learner	(mlr3::Learner) Learner to tune.
inner_resampli	ng
	(mlr3::Resampling)
	Resampling used for the inner loop.
outer_resampli	ng
	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	(bbotk::Terminator) Stop criterion of the tuning process.
search_space	(paradox::ParamSet) Hyperparameter search space. If NULL (default), the search space is constructed from the paradox::TuneToken of the learner's parameter set (learner\$param_set).
<pre>store_tuning_in</pre>	stance
	(logical(1)) If TRUE (default), stores the internally created TuningInstanceBatchSingleCrit with all intermediate results in slot \$tuning_instance.
store_benchmark	_result
	(logical(1)) If TRUE (default), store resample result of evaluated hyperparameter configura- tions in archive as mlr3::BenchmarkResult.
store_models	<pre>(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.</pre>
check_values	(logical(1)) If TRUE, hyperparameter values are checked before evaluation and performance scores after. If FALSE (default), values are unchecked but computational over- head is reduced.
callbacks	(list of mlr3misc::Callback) List of callbacks.

## 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()
```

TuningInstanceAsyncMultiCrit

Multi-Criteria Tuning with Rush

## Description

The TuningInstanceAsyncMultiCrit specifies a tuning problem for a Tuner. The function ti\_async() creates a TuningInstanceAsyncMultiCrit and the function tune() creates an instance internally.

#### Details

The instance contains an ObjectiveTuningAsync 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\_async()). This operation is usually done by the Tuner. Hyperparameter configurations are asynchronously sent to workers and evaluated by calling mlr3::resample(). The evaluated hyperparameter configurations are stored in the ArchiveAsyncTuning (\$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 ArchiveAsyncTuning to as.data.table(). The returned data table contains the mlr3::ResampleResult for each hyperparameter evaluation.

## Super classes

bbotk::OptimInstance->bbotk::OptimInstanceAsync->bbotk::OptimInstanceAsyncMultiCrit
->TuningInstanceAsyncMultiCrit

## **Public fields**

internal\_search\_space (paradox::ParamSet) The search space containing those parameters that are internally optimized by the mlr3::Learner.

#### Active bindings

result\_learner\_param\_vals (list()) List of param values for the optimal learner call.

## Methods

## **Public methods:**

- TuningInstanceAsyncMultiCrit\$new()
- TuningInstanceAsyncMultiCrit\$assign\_result()
- TuningInstanceAsyncMultiCrit\$clone()

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

```
Usage:
TuningInstanceAsyncMultiCrit$new(
    task,
    learner,
    resampling,
    measures,
    terminator,
    search_space = NULL,
    store_benchmark_result = TRUE,
    store_models = FALSE,
    check_values = FALSE,
    callbacks = NULL,
    rush = NULL
)
```

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 (bbotk::Terminator)
```

Stop criterion of the tuning process.

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

Hyperparameter search space. If NULL (default), the search space is constructed from the paradox::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.

callbacks (list of mlr3misc::Callback)

List of callbacks.

rush (Rush)

If a rush instance is supplied, the tuning runs without batches.

**Method** assign\_result(): The TunerAsync writes the best found points and estimated performance values here (probably the Pareto set / front). For internal use.

```
Usage:
 TuningInstanceAsyncMultiCrit$assign_result(
    xdt,
   ydt,
   learner_param_vals = NULL,
 )
 Arguments:
 xdt (data.table::data.table())
     Hyperparameter values as data.table::data.table(). Each row is one configuration.
     Contains values in the search space. Can contain additional columns for extra information.
 ydt (numeric(1))
     Optimal outcomes, e.g. the Pareto front.
 learner_param_vals (List of named list()s)
     Fixed parameter values of the learner that are neither part of the
 ... (any)
     ignored.
Method clone(): The objects of this class are cloneable with this method.
 Usage:
 TuningInstanceAsyncMultiCrit$clone(deep = FALSE)
```

runinginstanceAsynchulticrit\$clone(deep = r

Arguments:

deep Whether to make a deep clone.

TuningInstanceAsyncSingleCrit

Single Criterion Tuning with Rush

## Description

The TuningInstanceAsyncSingleCrit specifies a tuning problem for a TunerAsync. The function ti\_async() creates a TuningInstanceAsyncSingleCrit and the function tune() creates an instance internally.

#### Details

The instance contains an ObjectiveTuningAsync 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\_async()). This operation is usually done by the Tuner. Hyperparameter configurations are asynchronously sent to workers and evaluated by calling mlr3::resample(). The evaluated hyperparameter configurations are stored in the ArchiveAsyncTuning (\$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

## Analysis

For analyzing the tuning results, it is recommended to pass the ArchiveAsyncTuning to as.data.table(). The returned data table contains the mlr3::ResampleResult for each hyperparameter evaluation.

#### 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.

#### Super classes

```
bbotk::OptimInstance->bbotk::OptimInstanceAsync->bbotk::OptimInstanceAsyncSingleCrit
->TuningInstanceAsyncSingleCrit
```

## **Public fields**

internal\_search\_space (paradox::ParamSet) The search space containing those parameters that are internally optimized by the mlr3::Learner.

## Active bindings

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

## Methods

#### **Public methods:**

- TuningInstanceAsyncSingleCrit\$new()
- TuningInstanceAsyncSingleCrit\$assign\_result()
- TuningInstanceAsyncSingleCrit\$clone()

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

```
Usage:
TuningInstanceAsyncSingleCrit$new(
    task,
    learner,
    resampling,
    measure = NULL,
    terminator,
    search_space = NULL,
    store_benchmark_result = TRUE,
    store_models = FALSE,
    check_values = FALSE,
    callbacks = NULL,
    rush = NULL
)
Arguments:
```

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```
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 (bbotk::Terminator)
```

Stop criterion of the tuning process.

#### search\_space (paradox::ParamSet)

Hyperparameter search space. If NULL (default), the search space is constructed from the paradox::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.

callbacks (list of mlr3misc::Callback)

List of callbacks.

```
rush (Rush)
```

If a rush instance is supplied, the tuning runs without batches.

**Method** assign\_result(): The TunerAsync object writes the best found point and estimated performance value here. For internal use.

```
Usage:
TuningInstanceAsyncSingleCrit$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
    ... (any)
    ignored.
```

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

Usage:

TuningInstanceAsyncSingleCrit\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

TuningInstanceBatchMultiCrit

Class for Multi Criteria Tuning

#### Description

The TuningInstanceBatchMultiCrit specifies a tuning problem for a Tuner. The function ti() creates a TuningInstanceBatchMultiCrit and the function tune() creates an instance internally.

## Details

The instance contains an ObjectiveTuningBatch 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 ArchiveBatchTuning (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.

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#### Analysis

For analyzing the tuning results, it is recommended to pass the ArchiveBatchTuning 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::OptimInstanceBatch->bbotk::OptimInstanceBatchMultiCrit
->TuningInstanceBatchMultiCrit

## **Public fields**

internal\_search\_space (paradox::ParamSet)

The search space containing those parameters that are internally optimized by the mlr3::Learner.

## Active bindings

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

#### Methods

#### **Public methods:**

- TuningInstanceBatchMultiCrit\$new()
- TuningInstanceBatchMultiCrit\$assign\_result()
- TuningInstanceBatchMultiCrit\$clone()

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

## Usage:

```
TuningInstanceBatchMultiCrit$new(
   task,
   learner,
   resampling,
   measures,
   terminator,
   search_space = NULL,
   store_benchmark_result = TRUE,
   store_models = FALSE,
   check_values = FALSE,
   callbacks = NULL
)
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 (bbotk::Terminator)

Stop criterion of the tuning process.

search\_space (paradox::ParamSet)

Hyperparameter search space. If NULL (default), the search space is constructed from the paradox::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.

callbacks (list of mlr3misc::Callback) List of callbacks.

**Method** assign\_result(): The Tuner object writes the best found points and estimated performance values here. For internal use.

## Usage:

```
TuningInstanceBatchMultiCrit$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

... (any)

ignored.

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

Usage:

TuningInstanceBatchMultiCrit\$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 = rsmp("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)
```

```
TuningInstanceBatchSingleCrit
Class for Single Criterion Tuning
```

## Description

The TuningInstanceBatchSingleCrit specifies a tuning problem for a Tuner. The function ti() creates a TuningInstanceBatchSingleCrit and the function tune() creates an instance internally.

## Details

The instance contains an ObjectiveTuningBatch 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 ArchiveBatchTuning (\$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.

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#### Analysis

For analyzing the tuning results, it is recommended to pass the ArchiveBatchTuning 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::OptimInstanceBatch->bbotk::OptimInstanceBatchSingleCrit
->TuningInstanceBatchSingleCrit

## **Public fields**

internal\_search\_space (paradox::ParamSet)

The search space containing those parameters that are internally optimized by the mlr3::Learner.

## Active bindings

result\_learner\_param\_vals (list()) Param values for the optimal learner call.

#### Methods

#### **Public methods:**

- TuningInstanceBatchSingleCrit\$new()
- TuningInstanceBatchSingleCrit\$assign\_result()
- TuningInstanceBatchSingleCrit\$clone()

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

#### Usage:

```
TuningInstanceBatchSingleCrit$new(
   task,
   learner,
   resampling,
   measure = NULL,
   terminator,
   search_space = NULL,
   store_benchmark_result = TRUE,
   store_models = FALSE,
   check_values = FALSE,
   callbacks = NULL
)
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 (bbotk::Terminator)
```

Stop criterion of the tuning process.

#### search\_space (paradox::ParamSet)

Hyperparameter search space. If NULL (default), the search space is constructed from the paradox::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.

callbacks (list of mlr3misc::Callback)

List of callbacks.

**Method** assign\_result(): The Tuner object writes the best found point and estimated performance value here. For internal use.

```
Usage:
```

```
TuningInstanceBatchSingleCrit$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
```

... (any) ignored.

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

Usage:

TuningInstanceBatchSingleCrit\$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 = rsmp("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)
```

#### TuningInstanceMultiCrit

Multi Criteria Tuning Instance for Batch Tuning

## Description

TuningInstanceMultiCrit is a deprecated class that is now a wrapper around TuningInstance-BatchMultiCrit.

#### Super classes

```
bbotk::OptimInstance->bbotk::OptimInstanceBatch->bbotk::OptimInstanceBatchMultiCrit
->mlr3tuning::TuningInstanceBatchMultiCrit ->TuningInstanceMultiCrit
```

### Methods

#### **Public methods:**

- TuningInstanceMultiCrit\$new()
- 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,
   callbacks = NULL
)
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 (bbotk::Terminator)

Stop criterion of the tuning process.

#### search\_space (paradox::ParamSet)

Hyperparameter search space. If NULL (default), the search space is constructed from the paradox::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.

callbacks (list of mlr3misc::Callback)

List of callbacks.

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

Usage:

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

Arguments:

deep Whether to make a deep clone.

TuningInstanceSingleCrit

Single Criterion Tuning Instance for Batch Tuning

## Description

TuningInstanceSingleCrit is a deprecated class that is now a wrapper around TuningInstance-BatchSingleCrit.

## Super classes

bbotk::OptimInstance->bbotk::OptimInstanceBatch->bbotk::OptimInstanceBatchSingleCrit
->mlr3tuning::TuningInstanceBatchSingleCrit ->TuningInstanceSingleCrit

#### Methods

**Public methods:** 

- TuningInstanceSingleCrit\$new()
- 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,
   callbacks = NULL
)
```

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 (bbotk::Terminator)

Stop criterion of the tuning process.

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

Hyperparameter search space. If NULL (default), the search space is constructed from the paradox::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.

callbacks (list of mlr3misc::Callback)

List of callbacks.

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

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## TuningInstanceSingleCrit

Usage: TuningInstanceSingleCrit\$clone(deep = FALSE) Arguments: deep Whether to make a deep clone.

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