Package 'mlr3tuning'

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Title Tuning for 'mlr3'

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Description Implements methods for hyperparameter tuning with 'mlr3', e.g. grid search, random search, generalized simulated annealing and iterated racing. Various termination criteria can be set and combined. The class 'AutoTuner' provides a convenient way to perform nested resampling in combination with 'mlr3'.

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

Description

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Implements methods for hyperparameter tuning with 'mlr3', e.g. grid search, random search, generalized simulated annealing and iterated racing. Various termination criteria can be set and combined. The class 'AutoTuner' provides a convenient way to perform nested resampling in combination with 'mlr3'.

ArchiveTuning

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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

ArchiveTuning	Logging Object for	Evaluated Hyperparameter	Configurations
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Description

Container around a data.table::data.table() which stores all evaluated hyperparameter configurations and performance scores.

Data structure

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

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

Each row corresponds to a single evaluation of a hyperparameter configuration.

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 results are viewed with as.data.table(), both are joined automatically.

Analysis

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

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

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

The mlr3viz package provides visualizations for tuning results.

S3 Methods

 as.data.table.ArchiveTuning(x, unnest = "x_domain", exclude_columns = "uhash", measures = NULL)

Returns a tabular view of all evaluated hyperparameter configurations. ArchiveTuning -> data.table::data.table()

- x (ArchiveTuning)
- unnest (character()) Transforms list columns to separate columns. Set to NULL if no column should be unnested.
- exclude_columns (character())
 Exclude columns from table. Set to NULL if no column should be excluded.
- measures (List of mlr3::Measure)
 Score hyperparameter configurations on additional measures.

Super class

bbotk::Archive -> ArchiveTuning

Public fields

benchmark_result (mlr3::BenchmarkResult).

Methods

Public methods:

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

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

Usage:

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

Arguments:

search_space (paradox::ParamSet)

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

codomain (bbotk::Codomain)

Specifies codomain of objective function i.e. a set of performance measures. Internally created from provided mlr3::Measures.

```
check_values (logical(1))
```

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

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

```
Usage:
```

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

```
Arguments:

i (integer(1))

The iteration value to filter for.

uhash (logical(1))

The uhash value to filter for.
```

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

```
Usage:
ArchiveTuning$learners(i = NULL, uhash = NULL)
Arguments:
i (integer(1))
The iteration value to filter for.
uhash (logical(1))
The uhash value to filter for.
```

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

```
Usage:
ArchiveTuning$learner_param_vals(i = NULL, uhash = NULL)
Arguments:
i (integer(1))
The iteration value to filter for.
uhash (logical(1))
The uhash value to filter for.
```

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

```
Usage:
ArchiveTuning$predictions(i = NULL, uhash = NULL)
Arguments:
i (integer(1))
The iteration value to filter for.
uhash (logical(1))
The uhash value to filter for.
```

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

```
Usage:
ArchiveTuning$resample_result(i = NULL, uhash = NULL)
Arguments:
i (integer(1))
The iteration value to filter for.
uhash (logical(1))
The uhash value to filter for.
```

Method print(): Printer.

```
Usage:
ArchiveTuning$print()
Arguments:
... (ignored).
```

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

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

as_search_space Convert to a 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, ...)
```

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AutoTuner

Arguments

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

Value

paradox::ParamSet.

AutoTuner AutoTuner

Description

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

- 1. The hyperparameters of the wrapped (inner) learner are trained on the training data via resampling. The tuning can be specified by providing a Tuner, a bbotk::Terminator, a search space as paradox::ParamSet, a mlr3::Resampling and a mlr3::Measure.
- 2. The best found hyperparameter configuration is set as hyperparameters for the wrapped (inner) learner stored in at\$learner. Access the tuned hyperparameters via at\$learner\$param_set\$values.
- 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.

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

Super class

mlr3::Learner -> AutoTuner

Public fields

```
instance_args (list())
All arguments from construction to create the TuningInstanceSingleCrit.
tuners (Tean)
```

tuner (Tuner).

Active bindings

```
archive ArchiveTuning
Archive of the TuningInstanceSingleCrit.
```

learner (mlr3::Learner) Trained learner

tuning_instance (TuningInstanceSingleCrit) Internally created tuning instance with all intermediate results.

```
tuning_result (data.table::data.table)
    Short-cut to result from TuningInstanceSingleCrit.
```

predict_type (character(1))
 Stores the currently active predict type, e.g. "response". Must be an element of \$predict_types.

hash (character(1)) Hash (unique identifier) for this object.

Methods

Public methods:

- AutoTuner\$new()
- AutoTuner\$base_learner()
- AutoTuner\$print()
- AutoTuner\$clone()

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

```
Usage:
AutoTuner$new(
  learner,
  resampling,
  measure = NULL,
  terminator,
  tuner,
  search_space = NULL,
  store_tuning_instance = TRUE,
  store_benchmark_result = TRUE,
  store_models = FALSE,
  check_values = FALSE
)
```

.

Arguments:

learner (mlr3::Learner) Learner to tune, see TuningInstanceSingleCrit.

resampling (mlr3::Resampling)

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

measure (mlr3::Measure)

Performance measure to optimize.

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

When to stop tuning, see TuningInstanceSingleCrit.

```
tuner (Tuner)
```

Tuning algorithm to run.

search_space (paradox::ParamSet)

Hyperparameter search space. If NULL, the search space is constructed from the TuneToken in the ParamSet of the learner.

store_tuning_instance (logical(1))

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

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

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

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

```
check_values (logical(1))
```

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

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

Usage:

AutoTuner\$base_learner(recursive = Inf)

Arguments:

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

Returns: Learner. Printer.

Method print():

Usage:

AutoTuner\$print()

Arguments:

... (ignored).

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

Usage: AutoTuner\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

Examples

```
task = tsk("pima")
train_set = sample(task$nrow, 0.8 * task$nrow)
test_set = setdiff(seq_len(task$nrow), train_set)
at = AutoTuner$new(
  learner = lrn("classif.rpart", cp = to_tune(1e-04, 1e-1, logscale = TRUE)),
  resampling = rsmp("holdout"),
  measure = msr("classif.ce"),
  terminator = trm("evals", n_evals = 5),
  tuner = tnr("random_search"))
# tune hyperparameters and fit final model
at$train(task, row_ids = train_set)
# predict with final model
at$predict(task, row_ids = test_set)
# show tuning result
at$tuning_result
# model slot contains trained learner and tuning instance
at$model
# shortcut trained learner
at$learner
# shortcut tuning instance
at$tuning_instance
### nested resampling
at = AutoTuner$new(
  learner = lrn("classif.rpart", cp = to_tune(1e-04, 1e-1, logscale = TRUE)),
  resampling = rsmp("holdout"),
  measure = msr("classif.ce"),
  terminator = trm("evals", n_evals = 5),
  tuner = tnr("random_search"))
resampling_outer = rsmp("cv", folds = 3)
rr = resample(task, at, resampling_outer, store_models = TRUE)
# retrieve inner tuning results.
extract_inner_tuning_results(rr)
# performance scores estimated on the outer resampling
rr$score()
# unbiased performance of the final model trained on the full data set
rr$aggregate()
```

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auto_tuner

Description

Function to create an AutoTuner object.

Usage

```
auto_tuner(
  method,
  learner,
  resampling,
  measure = NULL,
  term_evals = NULL,
  term_time = NULL,
  search_space = NULL,
  store_models = FALSE,
  ...
)
```

Arguments

method	(character(1) Tuner) Key to retrieve tuner from mlr_tuners dictionary or Tuner object.
learner	(mlr3::Learner) Learner to tune.
resampling	(mlr3::Resampling) Resampling that is used to evaluated the performance of the hyperparameter configurations. Uninstantiated resamplings are instantiated during construction so that all configurations are evaluated on the same data splits. Already instanti- ated 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.
term_time	(integer(1)) Maximum allowed time in seconds.
search_space	(paradox::ParamSet) Hyperparameter search space. If NULL (default), the search space is constructed from the TuneToken of the learner's parameter set (learner\$param_set).

store_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>
	(named list()) Named arguments to be set as parameters of the tuner.

Value

AutoTuner

Examples

```
at = auto_tuner(
  method = "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"))

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 resample() or 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

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

```
at = auto_tuner(
  method = "grid_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_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. The function iterates over the AutoTuner objects and binds the tuning results to a data.table::data.table(). AutoTuner must be initialized with store_tuning_instance = TRUE and resample() or benchmark() must be called with store_models = TRUE.

Usage

extract_inner_tuning_results(x)

Arguments

Х

(mlr3::ResampleResult | mlr3::BenchmarkResult).

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

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mlr_tuners

Examples

```
learner = lrn("classif.rpart", cp = to_tune(1e-04, 1e-1, logscale = TRUE))
at = auto_tuner(
    method = "grid_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_tuning_results(rr)
```

mlr_tuners Dictionary of Tuners

Description

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

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

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

Format

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

Methods

See mlr3misc::Dictionary.

S3 methods

• as.data.table(dict, ..., objects = FALSE)

```
mlr3misc::Dictionary -> data.table::data.table()
```

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

See Also

Sugar functions: tnr(), tnrs()

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

Examples

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

mlr_tuners_cmaes Hyperparameter Tuning with Covariance Matrix Adaptation Evolution Strategy

Description

Subclass that implements CMA-ES calling adagio::pureCMAES() from package adagio.

Dictionary

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

```
TunerCmaes$new()
mlr_tuners$get("cmaes")
tnr("cmaes")
```

Parameters

```
sigma 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 adagio::pureCMAES(). Note that we have removed all control parameters which refer to the termination of the algorithm and where our terminators allow to obtain the same behavior.

Progress Bars

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

Logging

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

Optimizer

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

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Super classes

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

Methods

Public methods:

- TunerCmaes\$new()
- TunerCmaes\$clone()

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

Usage:

TunerCmaes\$new()

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

Usage:

TunerCmaes\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

Source

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

See Also

Package mlr3hyperband for hyperband tuning.

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

Examples

```
library(data.table)
# retrieve task
task = tsk("pima")
# 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))
)
# hyperparameter tuning on the pima indians diabetes data set
instance = tune(
    method = "cmaes",
    task = task,
    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(task)
```

mlr_tuners_design_points

Hyperparameter Tuning with via 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 via the dictionary mlr_tuners or with the associated sugar function tnr():

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

Parallelization

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

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

Logging

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

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Optimizer

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

Parameters

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

```
design data.table::data.table
```

Design points to try in search, one per row.

Progress Bars

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

Super classes

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

Methods

Public methods:

- TunerDesignPoints\$new()
- TunerDesignPoints\$clone()

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

Usage:

TunerDesignPoints\$new()

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

Usage:

TunerDesignPoints\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

See Also

Package mlr3hyperband for hyperband tuning.

Other Tuner: mlr_tuners_cmaes, mlr_tuners_gensa, mlr_tuners_grid_search, mlr_tuners_irace, mlr_tuners_nloptr, mlr_tuners_random_search, mlr_tuners

Examples

```
library(data.table)
# 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(
 method = "design_points",
 task = task,
 learner = learner,
 resampling = rsmp("holdout"),
 measure = msr("classif.ce"),
 design = data.table(cp = c(log(1e-1), log(1e-2)))
)
# 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_gensa Hyperparameter Tuning with Generalized Simulated Annealing

Description

Subclass for generalized simulated annealing tuning calling GenSA::GenSA() from package GenSA.

Dictionary

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

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

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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::OptimizerGenSA which can be applied on any black box optimization problem. See also the documentation of bbotk.

Parameters

smooth logical(1)

temperature numeric(1)

acceptance.param numeric(1)

verbose logical(1)

trace.mat logical(1)

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

Progress Bars

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

Super classes

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

Methods

Public methods:

- TunerGenSA\$new()
- TunerGenSA\$clone()

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

Usage: TunerGenSA\$new()

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

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

Source

Tsallis C, Stariolo DA (1996). "Generalized simulated annealing." *Physica A: Statistical Mechanics and its Applications*, **233**(1-2), 395–406. doi: 10.1016/s03784371(96)002713.

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

See Also

Package mlr3hyperband for hyperband tuning.

Other Tuner: mlr_tuners_cmaes, mlr_tuners_design_points, mlr_tuners_grid_search, mlr_tuners_irace, mlr_tuners_nloptr, mlr_tuners_random_search, mlr_tuners

Examples

```
# 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(
 method = "gensa",
 task = task,
 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(task)
```

mlr_tuners_grid_search

Hyperparameter Tuning with Grid Search

Description

Subclass for grid search tuning.

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 via the dictionary mlr_tuners or with the associated sugar function tnr():

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

Parameters

```
resolution integer(1)
    Resolution of the grid, see paradox::generate_design_grid().
```

```
param_resolutions named integer()
```

Resolution per parameter, named by parameter ID, see paradox::generate_design_grid().

```
batch_size integer(1)
```

Maximum number of points to try in a batch.

Progress Bars

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

Parallelization

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

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

Logging

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

Optimizer

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

Super class

mlr3tuning::Tuner -> TunerGridSearch

Methods

Public methods:

- TunerGridSearch\$new()
- TunerGridSearch\$clone()

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

Usage:

TunerGridSearch\$new()

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

Usage:

TunerGridSearch\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

See Also

Package mlr3hyperband for hyperband tuning.

Other Tuner: mlr_tuners_cmaes, mlr_tuners_design_points, mlr_tuners_gensa, mlr_tuners_irace, mlr_tuners_nloptr, mlr_tuners_random_search, mlr_tuners

Examples

```
# 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(
    method = "grid_search",
    task = task,
    learner = learner,
```

mlr_tuners_irace

```
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(task)
```

mlr_tuners_irace Tuning via Iterated Racing.

Description

TunerIrace class that implements iterated racing. Calls irace::irace() from package irace.

Dictionary

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

```
TunerIrace$new()
mlr_tuners$get("irace")
tnr("irace")
```

Parameters

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

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

Archive

The ArchiveTuning holds the following additional columns:

- "race" (integer(1)) Race iteration.
- "step" (integer(1)) Step number of race.

- "instance" (integer (1)) Identifies resampling instances across races and steps.
- "configuration" (integer(1)) Identifies configurations across races and steps.

Result

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

Progress Bars

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

Logging

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

Optimizer

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

Super classes

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

Methods

Public methods:

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

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

Usage:

TunerIrace\$new()

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

Usage: TunerIrace\$optimize(inst)
Arguments:

inst (TuningInstanceSingleCrit).

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mlr_tuners_irace

Returns: data.table::data.table.

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

Usage: TunerIrace\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

Source

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

See Also

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

Examples

```
# retrieve task
task = tsk("pima")
# load learner and set search space
learner = lrn("classif.rpart", cp = to_tune(1e-04, 1e-1, logscale = TRUE))
# hyperparameter tuning on the pima indians diabetes data set
instance = tune(
  method = "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

Description

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

Details

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

Dictionary

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

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

Logging

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

Optimizer

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

Parameters

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

start_values character(1)

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

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

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

Progress Bars

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

Super classes

mlr3tuning::Tuner -> mlr3tuning::TunerFromOptimizer -> TunerNLoptr

Methods

Public methods:

- TunerNLoptr\$new()
- TunerNLoptr\$clone()

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

Usage: TunerNLoptr\$new()

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

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

Source

Johnson, G S (2020). "The NLopt nonlinear-optimization package." https://github.com/stevengj/ nlopt.

See Also

Package mlr3hyperband for hyperband tuning.

Other Tuner: mlr_tuners_cmaes, mlr_tuners_design_points, mlr_tuners_gensa, mlr_tuners_grid_search, mlr_tuners_irace, mlr_tuners_random_search, mlr_tuners

Examples

```
## Not run:
# 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(
  method = "nloptr",
  task = task,
 learner = learner,
  resampling = rsmp("holdout"),
  measure = msr("classif.ce"),
  algorithm = "NLOPT_LN_BOBYQA"
)
# 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)
## End(Not run)
```

 ${\tt mlr_tuners_random_search}$

Hyperparameter Tuning with Random Search

Description

Subclass for random search tuning.

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

Dictionary

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

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

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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::OptimizerRandomSearch which can be applied on any black box optimization problem. See also the documentation of bbotk.

Parameters

```
batch_size integer(1)
```

Maximum number of points to try in a batch.

Progress Bars

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

Super classes

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

Methods

Public methods:

- TunerRandomSearch\$new()
- TunerRandomSearch\$clone()

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

Usage:

TunerRandomSearch\$new()

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

Usage:

TunerRandomSearch\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

Source

Bergstra J, Bengio Y (2012). "Random Search for Hyper-Parameter Optimization." *Journal of Machine Learning Research*, **13**(10), 281–305. https://jmlr.csail.mit.edu/papers/v13/bergstra12a.html.

See Also

Package mlr3hyperband for hyperband tuning.

Other Tuner: mlr_tuners_cmaes, mlr_tuners_design_points, mlr_tuners_gensa, mlr_tuners_grid_search, mlr_tuners_irace, mlr_tuners_nloptr, mlr_tuners

Examples

```
# 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(
 method = "random_search",
 task = task,
 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(task)
```

ObjectiveTuning ObjectiveTuning

Description

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

ObjectiveTuning

Super class

bbotk::Objective -> ObjectiveTuning

Public fields

task (mlr3::Task). learner (mlr3::Learner). resampling (mlr3::Resampling). measures (list of mlr3::Measure). store_models (logical(1)). store_benchmark_result (logical(1)). archive (ArchiveTuning). hotstart_stack (mlr3::HotstartStack). allow_hotstart (logical(1)). keep_hotstart_stack (logical(1)).

Methods

Public methods:

- ObjectiveTuning\$new()
- ObjectiveTuning\$clone()

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

```
Usage:
ObjectiveTuning$new(
    task,
    learner,
    resampling,
    measures,
    store_benchmark_result = TRUE,
    store_models = FALSE,
    check_values = TRUE,
    allow_hotstart = FALSE,
    keep_hotstart_stack = FALSE,
    archive = NULL
)
Arguments:
```

task (mlr3::Task) Task to operate on. learner (mlr3::Learner) Learner to tune. resampling (mlr3::Resampling)

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

measures (list of mlr3::Measure)

Measures to optimize.

```
store_benchmark_result (logical(1))
```

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

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

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

```
check_values (logical(1))
```

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

allow_hotstart (logical(1))

Allow to hotstart learners with previously fitted models. See also mlr3::HotstartStack. The learner must support hotstarting. Sets store_models = TRUE.

```
keep_hotstart_stack (logical(1))
```

If TRUE, mlr3::HotstartStack is kept in \$objective\$hotstart_stack after tuning.

archive (ArchiveTuning)

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

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.

tnr

Syntactic Sugar for Tuner Construction

Description

This function complements mlr_tuners with functions in the spirit of mlr3::mlr_sugar.

Usage

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

tune

Arguments

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

Value

- Tuner for tnr()
- list of Tuner for tnrs()

Examples

tnr("random_search")

tune

Function for Tuning

Description

Function to tune a mlr3::Learner.

Usage

```
tune(
  method,
  task,
  learner,
  resampling,
  measures = NULL,
  term_evals = NULL,
  term_time = NULL,
  search_space = NULL,
  store_models = FALSE,
  allow_hotstart = FALSE,
  keep_hotstart_stack = FALSE,
  ...
)
```

Arguments

method	(character(1) Tuner) Key to retrieve tuner from mlr_tuners dictionary or Tuner object.
task	(mlr3::Task) Task to operate on.
learner	(mlr3::Learner) Learner to tune.
resampling	(mlr3::Resampling) Resampling that is used to evaluated the performance of the hyperparameter configurations. Uninstantiated resamplings are instantiated during construction so that all configurations are evaluated on the same data splits. Already instanti- ated 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.
term_evals	(integer(1)) Number of allowed evaluations.
term_time	(integer(1)) Maximum allowed time in seconds.
search_space	(paradox::ParamSet) Hyperparameter search space. If NULL (default), the search space is constructed from the TuneToken of the learner's parameter set (learner\$param_set).
store_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>
allow_hotstart	(logical(1)) Allow to hotstart learners with previously fitted models. See also mlr3::HotstartStack. The learner must support hotstarting. Sets store_models = TRUE.
keep_hotstart_s	tack
	<pre>(logical(1)) If TRUE, mlr3::HotstartStack is kept in \$objective\$hotstart_stack after tun- ing.</pre>
	(named list()) Named arguments to be set as parameters of the tuner.

Value

TuningInstanceSingleCrit | TuningInstanceMultiCrit

Examples

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

Tuner

```
instance = tune(
  method = "random_search",
  task = tsk("pima"),
  learner = learner,
  resampling = rsmp ("holdout"),
  measures = msr("classif.ce"),
  term_evals = 4)
# apply hyperparameter values to learner
learner$param_set$values = instance$result_learner_param_vals
```

Tuner

Tuner

Description

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

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

Private Methods

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

Technical Details and Subclasses

A subclass is implemented in the following way:

- Inherit from Tuner.
- Specify the private abstract method \$.tune() and use it to call into your optimizer.
- You need to call instance\$eval_batch() to evaluate design points.
- The batch evaluation is requested at the TuningInstanceSingleCrit/TuningInstanceMultiCrit object instance, so each batch is possibly executed in parallel via mlr3::benchmark(), and all evaluations are stored inside of instance\$archive.
- Before the batch evaluation, the 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.

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. Subclasses of paradox::Param.

```
properties (character())
```

Set of properties of the tuner. Must be a subset of mlr_reflections\$tuner_properties.

packages (character())

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

```
label (character(1))
```

Label for this object. Can be used in tables, plot and text output instead of the ID.

man (character(1))

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

Methods

Public methods:

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

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

Usage:

Tuner

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

Method print(): Print method.

```
Usage:
Tuner$print()
Returns: (character()).
```

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

Usage: Tuner\$help()

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

Usage:

tune_nested

Tuner\$optimize(inst)
Arguments:
inst (TuningInstanceSingleCrit | TuningInstanceMultiCrit).
Returns: data.table::data.table

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

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

tune_nested Function for Nested Resampling

Description

Function to conduct nested resampling.

Usage

```
tune_nested(
  method,
  task,
  learner,
  inner_resampling,
  outer_resampling,
  measure = NULL,
  term_evals = NULL,
  term_time = NULL,
  search_space = NULL,
  ...
)
```

Arguments

(character(1)) Key to retrieve tuner from mlr_tuners dictionary.
(mlr3::Task) Task to operate on.
(mlr3::Learner) Learner to tune.
g
(mlr3::Resampling)
Resampling used for the inner loop.

TuningInstanceMultiCrit

outer_resamplir	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.
term_time	(integer(1)) Maximum allowed time in seconds.
search_space	(paradox::ParamSet) Hyperparameter search space. If NULL (default), the search space is constructed from the TuneToken of the learner's parameter set (learner\$param_set).
	(named list()) Named arguments to be set as parameters of the tuner.

Value

mlr3::ResampleResult

Examples

```
rr = tune_nested(
    method = "random_search",
    task = tsk("pima"),
    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,
    batch_size = 2)
# 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()
```

 ${\tt TuningInstance} {\tt MultiCrit}$

Multi Criteria Tuning Instance

Description

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

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

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

Super classes

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

Active bindings

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

Methods

Public methods:

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

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

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

Usage:

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

```
task (mlr3::Task)
```

Task to operate on.

learner (mlr3::Learner)

Learner to tune.

resampling (mlr3::Resampling)

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

measures (list of mlr3::Measure)

Measures to optimize.

```
terminator (Terminator)
```

Stop criterion of the tuning process.

search_space (paradox::ParamSet)

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

store_benchmark_result (logical(1))

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

store_models (logical(1))

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

check_values (logical(1))

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

allow_hotstart (logical(1))

Allow to hotstart learners with previously fitted models. See also mlr3::HotstartStack. The learner must support hotstarting. Sets store_models = TRUE.

```
keep_hotstart_stack (logical(1))
```

If TRUE, mlr3::HotstartStack is kept in \$objective\$hotstart_stack after tuning.

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

Usage:

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

Arguments:

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

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

ydt (data.table::data.table())

Optimal outcomes, e.g. the Pareto front.

learner_param_vals (List of named list()s)

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

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

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

Examples

```
library(data.table)
```

```
# define search space
search_space = ps(
 cp = p_dbl(lower = 0.001, upper = 0.1),
 minsplit = p_int(lower = 1, upper = 10)
)
# initialize instance
instance = TuningInstanceMultiCrit$new(
 task = tsk("iris"),
 learner = lrn("classif.rpart"),
 resampling = rsmp("holdout"),
 measure = msrs(c("classif.ce", "classif.acc")),
 search_space = search_space,
 terminator = trm("evals", n_evals = 5)
)
# generate design
design = data.table(cp = c(0.05, 0.01), minsplit = c(5, 3))
# eval design
instance$eval_batch(design)
# show archive
instance$archive
```

TuningInstanceSingleCrit

Single Criterion Tuning Instance

Description

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

Evaluations of hyperparameter configurations are performed in batches by calling mlr3::benchmark() internally. Before a batch is evaluated, the bbotk::Terminator is queried for the remaining budget.

TuningInstanceSingleCrit

If the available budget is exhausted, an exception is raised, and no further evaluations can be performed from this point on.

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

Super classes

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

Active bindings

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

Methods

Public methods:

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

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

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

```
Usage:
TuningInstanceSingleCrit$new(
   task,
   learner,
   resampling,
   measure = NULL,
   terminator,
   search_space = NULL,
   store_benchmark_result = TRUE,
   store_models = FALSE,
   check_values = FALSE,
   allow_hotstart = FALSE,
   keep_hotstart_stack = FALSE
)
Arguments:
```

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

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

Learner to tune.

```
resampling (mlr3::Resampling)
```

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

measure (mlr3::Measure)

Measure to optimize. If NULL, default measure is used.

terminator (Terminator)

Stop criterion of the tuning process.

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

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

```
store_benchmark_result (logical(1))
```

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

store_models (logical(1))

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

check_values (logical(1))

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

allow_hotstart (logical(1))

Allow to hotstart learners with previously fitted models. See also mlr3::HotstartStack. The learner must support hotstarting. Sets store_models = TRUE.

keep_hotstart_stack (logical(1))

If TRUE, mlr3::HotstartStack is kept in \$objective\$hotstart_stack after tuning.

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

Usage:

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

Arguments:

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

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

y (numeric(1))

Optimal outcome.

learner_param_vals (List of named list()s)

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

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

Usage:

TuningInstanceSingleCrit\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

TuningInstanceSingleCrit

Examples

```
library(data.table)
# define search space
search_space = ps(
  cp = p_dbl(lower = 0.001, upper = 0.1),
  minsplit = p_int(lower = 1, upper = 10)
)
# initialize instance
instance = TuningInstanceSingleCrit$new(
  task = tsk("iris"),
  learner = lrn("classif.rpart"),
  resampling = rsmp("holdout"),
  measure = msr("classif.ce"),
  search_space = search_space,
  terminator = trm("evals", n_evals = 5)
)
# generate design
design = data.table(cp = c(0.05, 0.01), minsplit = c(5, 3))
# eval design
instance$eval_batch(design)
# show archive
instance$archive
### error handling
# get a learner which breaks with 50% probability
# set encapsulation + fallback
learner = lrn("classif.debug", error_train = 0.5)
learner$encapsulate = c(train = "evaluate", predict = "evaluate")
learner$fallback = lrn("classif.featureless")
# define search space
search_space = ps(
x = p_dbl(lower = 0, upper = 1)
)
instance = TuningInstanceSingleCrit$new(
  task = tsk("wine"),
  learner = learner,
  resampling = rsmp("cv", folds = 3),
  measure = msr("classif.ce"),
  search_space = search_space,
  terminator = trm("evals", n_evals = 5)
)
instance$eval_batch(data.table(x = 1:5 / 5))
```

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