Package 'bbotk'

September 13, 2021

Title Black-Box Optimization Toolkit

Version 0.4.0

Description Provides a common framework for optimization of black-box functions for other packages, e.g. 'mlr3tuning' or 'mlr3fselect'. It offers various optimization methods e.g. grid search, random search, generalized simulated annealing and iterated racing.

License LGPL-3

URL https://bbotk.mlr-org.com, https://github.com/mlr-org/bbotk

BugReports https://github.com/mlr-org/bbotk/issues

Depends paradox (>= 0.7.0), R (>= 3.1.0)

Imports checkmate (>= 2.0.0), data.table, lgr, methods, mlr3misc (>= 0.7.0), R6

Suggests adagio, GenSA, irace, knitr, nloptr, progressr, rmarkdown, testthat (>= 3.0.0)

VignetteBuilder knitr

Config/testthat/edition 3

Config/testthat/parallel false

Encoding UTF-8

Language en-US

NeedsCompilation yes

RoxygenNote 7.1.2

Collate 'Archive.R' 'ArchiveBest.R' 'Objective.R' 'ObjectiveRFun.R' 'ObjectiveRFunDt.R' 'OptimInstance.R' 'OptimInstanceMultiCrit.R' 'OptimInstanceSingleCrit.R' 'mlr_optimizers.R' 'Optimizer.R' 'OptimizerCmaes.R' 'OptimizerDesignPoints.R' 'OptimizerGenSA.R' 'OptimizerGridSearch.R' 'OptimizerIrace.R' 'OptimizerNLoptr.R' 'OptimizerRandomSearch.R' 'Progressor.R' 'mlr_terminators.R' 'Terminator.R' 'TerminatorClockTime.R' 'TerminatorCombo.R' 'TerminatorEvals.R' 'TerminatorNone.R'

'TerminatorPerfReached.R' 'TerminatorRunTime.R'
'TerminatorStagnation.R' 'TerminatorStagnationBatch.R'
'assertions.R' 'bb_optimize.R' 'bbotk_reflections.R'
'bibentries.R' 'helper.R' 'helper_irace.R' 'sugar.R' 'zzz.R'

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

Maintainer Marc Becker <marcbecker@posteo.de>

Repository CRAN

Date/Publication 2021-09-13 15:50:08 UTC

R topics documented:

---

bbotk-package *bbotk: Black-Box Optimization Toolkit*

Description

Provides a common framework for optimization of black-box functions for other packages, e.g. 'mlr3tuning' or 'mlr3fselect'. It offers various optimization methods e.g. grid search, random search, generalized simulated annealing and iterated racing.

Author(s)

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

Authors:

- Jakob Richter <jakob1richter@gmail.com> (ORCID)
- Michel Lang <michellang@gmail.com> (ORCID)
- Bernd Bischl <bernd_bischl@gmx.net> (ORCID)
- Martin Binder <martin.binder@mail.com>

Other contributors:

- Olaf Mersmann <olafm@statistik.tu-dortmund.de> [contributor]

See Also

Useful links:

- https://bbotk.mlr-org.com
- https://github.com/mlr-org/bbotk
- Report bugs at https://github.com/mlr-org/bbotk/issues

`Archive` *Logging object for objective function evaluations*

Description

Container around a data.table::data.table which stores all performed function calls of the Objective.

S3 Methods

- `as.data.table(archive)`
  Archive -> `data.table::data.table()`
  Returns a tabular view of all performed function calls of the Objective. The `x_domain` column is unnested to separate columns.

Public fields

`search_space` (paradox::ParamSet)
: Search space of objective.

`codomain` (paradox::ParamSet)
: Codomain of objective function.

`start_time` (POSIXct)
: Time stamp of when the optimization started. The time is set by the Optimizer.

`check_values` (`logical(1)`)
: Determines if points and results are checked for validity.

`data` (data.table::data.table)
: Contains all performed Objective function calls.

`store_x_domain` (`logical(1)`)
: Determines if x values, should be stored in $data$x_domain as list items. The trafo will be applied if defined in `search_space`.

Active bindings

`n_evals` (`integer(1)`)
: Number of evaluations stored in the archive.

`n_batch` (`integer(1)`)
: Number of batches stored in the archive.

`cols_x` (`character()`)
: Column names of search space parameters.

`cols_y` (`character()`)
: Column names of codomain parameters.

Methods

Public methods:

- Archive$new()
- Archive$add_evals()
- Archive$best()
- Archive$format()
- Archive$print()
- Archive$clear()
- Archive$clone()

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

Usage:

```
Archive$new(search_space, codomain, check_values = TRUE, store_x_domain = TRUE)
```

Arguments:

`search_space` (paradox::ParamSet)
: Specifies the search space for the Optimizer. The paradox::ParamSet describes either a subset of the `domain` of the Objective or it describes a set of parameters together with a `trafo` function that transforms values from the search space to values of the domain. Depending on the context, this value defaults to the domain of the objective.

`codomain` (paradox::ParamSet)
: Specifies codomain of function. Most importantly the tags of each output "Parameter" define whether it should be minimized or maximized. The default is to minimize each component.

`check_values` (`logical(1)`)
: Should x-values that are added to the archive be checked for validity? Search space that is logged into archive.

`store_x_domain` (`logical(1)`)
: Determines if x values, should be stored in $data$x_domain as list items. The trafo will be applied if defined in `search_space`.

Method `add_evals()`**:** Adds function evaluations to the archive table.

Usage:

```
Archive$add_evals(xdt, xss_trafoed = NULL, ydt)
```

Arguments:

`xdt` (`data.table::data.table()`)
: Set of untransformed points / points from the *search space*. One point per row, e.g. `data.table(x1 = c(1,3),x2 = c(2,4))`. Column names have to match ids of the `search_space`. However, `xdt` can contain additional columns.

`xss_trafoed` (`list()`)
: Transformed point(s) in the *domain space*. Not stored and needed if `store_x_domain = FALSE`.

`ydt` (`data.table::data.table()`)
: Optimal outcome.

Method `best()`**:** Returns the best scoring evaluation. For single-crit optimization, the solution that minimizes / maximizes the objective function. For multi-crit optimization, the Pareto set / front.

Usage:

```
Archive$best(batch = NULL)
```

Arguments:

`batch (integer())`
The batch number(s) to limit the best results to. Default is all batches.

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

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

Usage:

```
Archive$format()
```

Method `print()`**:** Printer.

Usage:

```
Archive$print()
```

Arguments:

`...` (ignored).

Method `clear()`**:** Clear all evaluation results from archive.

Usage:

```
Archive$clear()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

`ArchiveBest` *Minimal logging object for objective function evaluations*

Description

The ArchiveBest stores no data but records the best scoring evaluation passed to $add_evals(). The Archive API is fully implemented but many parameters are ignored and some methods do nothing. The archive still works with TerminatorClockTime, TerminatorEvals, TerminatorNone and TerminatorEvals.

Super class

`bbotk::Archive` -> `ArchiveBest`

Active bindings

`n_evals (integer(1))`
: Number of evaluations stored in the archive.

`n_batch (integer(1))`
: Number of batches stored in the archive.

Methods

Public methods:

- `ArchiveBest$new()`
- `ArchiveBest$add_evals()`
- `ArchiveBest$best()`
- `ArchiveBest$clone()`

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

Usage:

```
ArchiveBest$new(
  search_space,
  codomain,
  check_values = FALSE,
  store_x_domain = FALSE
)
```

Arguments:

`search_space` (paradox::ParamSet)
: Specifies the search space for the Optimizer. The paradox::ParamSet describes either a subset of the `domain` of the Objective or it describes a set of parameters together with a `trafo` function that transforms values from the search space to values of the domain. Depending on the context, this value defaults to the domain of the objective.

`codomain` (paradox::ParamSet)
: Specifies codomain of function. Most importantly the tags of each output "Parameter" define whether it should be minimized or maximized. The default is to minimize each component.

`check_values (logical(1))`
: ignored.

`store_x_domain (logical(1))`
: Determines if x values, should be stored in $data$x_domain as list items. The trafo will be applied if defined in `search_space`.

Method `add_evals()`**:** Stores the best result in `ydt`.

Usage:

```
ArchiveBest$add_evals(xdt, xss_trafoed = NULL, ydt)
```

Arguments:

`xdt` (`data.table::data.table()`)
: Set of untransformed points / points from the *search space*. One point per row, e.g. `data.table(x1 = c(1,3),x2 = c(2,4))`. Column names have to match ids of the `search_space`. However, `xdt` can contain additional columns.

`xss_trafoed` (`list()`)
Transformed point(s) in the *domain space*.

`ydt` (`data.table::data.table()`)
Optimal outcome.

Method `best()`**:** Returns the best scoring evaluation. For single-crit optimization, the solution that minimizes / maximizes the objective function. For multi-crit optimization, the Pareto set / front.

Usage:

```
ArchiveBest$best(m = NULL)
```

Arguments:

`m` (`integer()`)
ignored.

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

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

`bb_optimize` *Black-Box Optimization*

Description

This function optimizes a function or Objective with a given method.

Usage

```
bb_optimize(
  x,
  method = "random_search",
  max_evals = 1000,
  max_time = NULL,
  ...
)

## S3 method for class '`function`'
bb_optimize(
  x,
  method = "random_search",
  max_evals = 1000,
  max_time = NULL,
  lower = NULL,
```

```
  upper = NULL,
  maximize = FALSE,
  ...
)

## S3 method for class 'Objective'
bb_optimize(
  x,
  method = "random_search",
  max_evals = 1000,
  max_time = NULL,
  search_space = NULL,
  ...
)
```

Arguments

x	(function | Objective).
method	(character(1) | Optimizer) Key to retrieve optimizer from mlr_optimizers dictionary or Optimizer.
max_evals	(integer(1)) Number of allowed evaluations.
max_time	(integer(1)) Maximum allowed time in seconds.
...	(named list()) Named arguments passed to objective function. Ignored if Objective is optimized.
lower	(numeric()) Lower bounds on the parameters. If named, names are used to create the domain.
upper	(numeric()) Upper bounds on the parameters.
maximize	(logical()) Logical vector used to create the codomain e.g. c(TRUE, FALSE) -> ps(y1 = p_dbl(tags = "maximize"), y2 = pd_dbl(tags = "minimize")). If named, names are used to create the codomain.
search_space	(paradox::ParamSet).

Value

list of

- "par" - Best found parameters
- "value" - Optimal outcome
- "instance" - OptimInstanceSingleCrit | OptimInstanceMultiCrit

Note

If both `max_evals` and `max_time` are `NULL`, TerminatorNone is used. This is useful if the Optimizer can terminate itself. If both are given, TerminatorCombo is created and the optimization stops if the time or evaluation budget is exhausted.

Examples

```
# function and bounds
fun = function(xs) {
  - (xs[[1]] - 2)^2 - (xs[[2]] + 3)^2 + 10
}

bb_optimize(fun, lower = c(-10, -5), upper = c(10, 5), max_evals = 10)

# function and constant
fun = function(xs, c) {
  - (xs[[1]] - 2)^2 - (xs[[2]] + 3)^2 + c
}

bb_optimize(fun, lower = c(-10, -5), upper = c(10, 5), max_evals = 10, c = 1)

# objective
fun = function(xs) {
  c(z = - (xs[[1]] - 2)^2 - (xs[[2]] + 3)^2 + 10)
}

# define domain and codomain using a `ParamSet` from paradox
domain = ps(x1 = p_dbl(-10, 10), x2 = p_dbl(-5, 5))
codomain = ps(z = p_dbl(tags = "minimize"))
objective = ObjectiveRFun$new(fun, domain, codomain)

bb_optimize(objective, method = "random_search", max_evals = 10)
```

---

is_dominated *Calculate which points are dominated*

Description

Returns which points from a set are dominated by another point in the set.

Usage

```
is_dominated(ymat)
```

Arguments

`ymat`	(`matrix()`) A numeric matrix. Each column (!) contains one point.

mlr_optimizers *Dictionary of Optimizer*

Description

A simple mlr3misc::Dictionary storing objects of class Optimizer. Each optimizer has an associated help page, see `mlr_optimizer_[id]`.

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

For a more convenient way to retrieve and construct optimizer, see `opt()`/`opts()`.

Format

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

Methods

See mlr3misc::Dictionary.

See Also

Sugar functions: `opt()`, `opts()`

Examples

```
opt("random_search", batch_size = 10)
```

mlr_optimizers_cmaes *Optimization via Covariance Matrix Adaptation Evolution Strategy*

Description

`OptimizerCmaes` class that implements CMA-ES. Calls `adagio::pureCMAES()` from package **adagio**. The algorithm is typically applied to search space dimensions between three and fifty. Lower search space dimensions might crash.

Dictionary

This Optimizer can be instantiated via the dictionary mlr_optimizers or with the associated sugar function `opt()`:

```
mlr_optimizers$get("cmaes")
opt("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")`.

Super class

`bbotk::Optimizer` -> `OptimizerCmaes`

Methods

Public methods:

- `OptimizerCmaes$new()`
- `OptimizerCmaes$clone()`

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

Usage:

```
OptimizerCmaes$new()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Examples

```
if(requireNamespace("adagio")) {
search_space = domain = ps(
  x1 = p_dbl(-10, 10),
  x2 = p_dbl(-5, 5)
)

codomain = ps(y = p_dbl(tags = "maximize"))

objective_function = function(xs) {
  c(y = - (xs[[1]] - 2)^2 - (xs[[2]] + 3)^2 + 10)
}
```

```
objective = ObjectiveRFun$new(
  fun = objective_function,
  domain = domain,
  codomain = codomain)

instance = OptimInstanceSingleCrit$new(
  objective = objective,
  search_space = search_space,
  terminator = trm("evals", n_evals = 10))

optimizer = opt("cmaes")

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

# returns best scoring evaluation
instance$result

# allows access of data.table of full path of all evaluations
as.data.table(instance$archive$data)
}
```

`mlr_optimizers_design_points`

Optimization via Design Points

Description

`OptimizerDesignPoints` class that implements optimization 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.

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.

Dictionary

This Optimizer can be instantiated via the dictionary mlr_optimizers or with the associated sugar function `opt()`:

```
mlr_optimizers$get("design_points")
opt("design_points")
```

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 class

`bbotk::Optimizer` -> `OptimizerDesignPoints`

Methods

Public methods:

- `OptimizerDesignPoints$new()`
- `OptimizerDesignPoints$clone()`

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

Usage:

```
OptimizerDesignPoints$new()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Examples

```
library(data.table)
search_space = domain = ps(x = p_dbl(lower = -1, upper = 1))

codomain = ps(y = p_dbl(tags = "minimize"))

objective_function = function(xs) {
  list(y = as.numeric(xs)^2)
}

objective = ObjectiveRFun$new(
 fun = objective_function,
 domain = domain,
 codomain = codomain)

instance = OptimInstanceSingleCrit$new(
 objective = objective,
 search_space = search_space,
 terminator = trm("evals", n_evals = 10))

design = data.table(x = c(0, 1))

optimizer = opt("design_points", design = design)
```

```
# Modifies the instance by reference
optimizer$optimize(instance)

# Returns best scoring evaluation
instance$result

# Allows access of data.table of full path of all evaluations
as.data.table(instance$archive)
```

`mlr_optimizers_gensa` *Optimization via Generalized Simulated Annealing*

Description

`OptimizerGenSA` class that implements generalized simulated annealing. Calls `GenSA::GenSA()` from package **GenSA**.

Dictionary

This Optimizer can be instantiated via the dictionary mlr_optimizers or with the associated sugar function `opt()`:

```
mlr_optimizers$get("gensa")
opt("gensa")
```

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 class

`bbotk::Optimizer` -> `OptimizerGenSA`

Methods

Public methods:

- `OptimizerGenSA$new()`
- `OptimizerGenSA$clone()`

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

Usage:

```
OptimizerGenSA$new()
```

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

Usage:

```
OptimizerGenSA$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.

Examples

```
if(requireNamespace("GenSA")) {

search_space = domain = ps(x = p_dbl(lower = -1, upper = 1))

codomain = ps(y = p_dbl(tags = "minimize"))

objective_function = function(xs) {
  list(y = as.numeric(xs)^2)
}

objective = ObjectiveRFun$new(
 fun = objective_function,
 domain = domain,
 codomain = codomain)

instance = OptimInstanceSingleCrit$new(
 objective = objective,
 search_space = search_space,
 terminator = trm("evals", n_evals = 10))

optimizer = opt("cmaes")

# Modifies the instance by reference
optimizer$optimize(instance)
```

```
# Returns best scoring evaluation
instance$result

# Allows access of data.table of full path of all evaluations
as.data.table(instance$archive$data)
}
```

`mlr_optimizers_grid_search`

Optimization via Grid Search

Description

`OptimizerGridSearch` class that implements grid search. The grid is constructed as a Cartesian product over discretized values per parameter, see `paradox::generate_design_grid()`. The points of the grid are evaluated in a random order.

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.

Dictionary

This Optimizer can be instantiated via the dictionary mlr_optimizers or with the associated sugar function `opt()`:

```
mlr_optimizers$get("grid_search")
opt("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")`.

Super class

`bbotk::Optimizer` -> `OptimizerGridSearch`

Methods

Public methods:

- `OptimizerGridSearch$new()`
- `OptimizerGridSearch$clone()`

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

Usage:

```
OptimizerGridSearch$new()
```

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

Usage:

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

Arguments:

deep Whether to make a deep clone.

Examples

```
search_space = domain = ps(x = p_dbl(lower = -1, upper = 1))

codomain = ps(y = p_dbl(tags = "minimize"))

objective_function = function(xs) {
  list(y = as.numeric(xs)^2)
}

objective = ObjectiveRFun$new(
 fun = objective_function,
 domain = domain,
 codomain = codomain)

instance = OptimInstanceSingleCrit$new(
 objective = objective,
 search_space = search_space,
 terminator = trm("evals", n_evals = 10))


optimizer = opt("grid_search")

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

# returns best scoring evaluation
instance$result

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

`mlr_optimizers_irace` *Optimization via Iterated Racing*

Description

`OptimizerIrace` class that implements iterated racing. Calls `irace::irace()` from package **irace**.

Parameters

`instances list()`
: A list of instances where the configurations executed on.

`targetRunnerParallel function()`
: A function that executes the objective function with a specific parameter configuration and instance. A default function is provided, see section "Target Runner and 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 `OptimizerIrace`.

Target Runner and Instances

The irace package uses a `targetRunner` script or R function to evaluate a configuration on a particular instance. Usually it is not necessary to specify a `targetRunner` function when using `OptimizerIrace`. A default function is used that forwards several configurations and instances to the user defined objective function. As usually, the user defined function has a `xs`, `xss` or `xdt` parameter depending on the used Objective class. For irace, the function needs an additional `instances` parameter.

```
fun = function(xs, instances) {
 # function to evaluate configuration in `xs` on instance `instances`
}
```

Archive

The Archive holds the following additional columns:

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

Result

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

Dictionary

This Optimizer can be instantiated via the dictionary mlr_optimizers or with the associated sugar function `opt()`:

```
mlr_optimizers$get("irace")
opt("irace")
```

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 class

`bbotk::Optimizer` -> `OptimizerIrace`

Methods

Public methods:

- `OptimizerIrace$new()`
- `OptimizerIrace$clone()`

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

Usage:

```
OptimizerIrace$new()
```

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

Usage:

```
OptimizerIrace$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.

Examples

```
library(data.table)

search_space = domain = ps(
  x1 = p_dbl(-5, 10),
  x2 = p_dbl(0, 15)
)
```

```
codomain = ps(y = p_dbl(tags = "minimize"))

# branin function with noise
# the noise generates different instances of the branin function
# the noise values are passed via the `instances` parameter
fun = function(xdt, instances) {
  a = 1
  b = 5.1 / (4 * (pi ^ 2))
  c = 5 / pi
  r = 6
  s = 10
  t = 1 / (8 * pi)

  data.table(y = (
    a * ((xdt[["x2"]] -
    b * (xdt[["x1"]] ^ 2L) +
    c * xdt[["x1"]] - r) ^ 2) +
    ((s * (1 - t)) * cos(xdt[["x1"]])) +
    unlist(instances)))
}

objective = ObjectiveRFunDt$new(fun = fun, domain = domain,  codomain = codomain)

instance = OptimInstanceSingleCrit$new(
  objective = objective,
  search_space = search_space,
  terminator = trm("evals", n_evals = 1000))

# create instances of branin function
instances = rnorm(10, mean = 0, sd = 0.1)

# load optimizer irace and set branin instances
optimizer = opt("irace", instances = instances)

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

# best scoring configuration
instance$result

# all evaluations
as.data.table(instance$archive)
```

`mlr_optimizers_nloptr` *Optimization via Non-linear Optimization*

Description

`OptimizerNLoptr` class that implements non-linear optimization. Calls `nloptr::nloptr()` from package **nloptr**.

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 class

`bbotk::Optimizer` -> `OptimizerNLoptr`

Methods

Public methods:

- `OptimizerNLoptr$new()`
- `OptimizerNLoptr$clone()`

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

Usage:

```
OptimizerNLoptr$new()
```

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

Usage:

```
OptimizerNLoptr$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.

Examples

```
if(requireNamespace("nloptr")) {

search_space = domain = ps(x = p_dbl(lower = -1, upper = 1))

codomain = ps(y = p_dbl(tags = "minimize"))

objective_function = function(xs) {
  list(y = as.numeric(xs)^2)
}

objective = ObjectiveRFun$new(
 fun = objective_function,
 domain = domain,
 codomain = codomain)


# We use the internal termination criterion xtol_rel
terminator = trm("none")
instance = OptimInstanceSingleCrit$new(
 objective = objective,
 search_space = search_space,
 terminator = terminator)


optimizer = opt("nloptr", algorithm = "NLOPT_LN_BOBYQA")

# Modifies the instance by reference
optimizer$optimize(instance)

# Returns best scoring evaluation
instance$result

# Allows access of data.table of full path of all evaluations
as.data.table(instance$archive)
}
```

---

mlr_optimizers_random_search

Optimization via Random Search

Description

`OptimizerRandomSearch` class that implements a simple Random Search.

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.

Dictionary

This Optimizer can be instantiated via the dictionary mlr_optimizers or with the associated sugar function `opt()`:

```
mlr_optimizers$get("random_search")
opt("random_search")
```

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 class

`bbotk::Optimizer` -> `OptimizerRandomSearch`

Methods

Public methods:

- `OptimizerRandomSearch$new()`
- `OptimizerRandomSearch$clone()`

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

Usage:

```
OptimizerRandomSearch$new()
```

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

Usage:

```
OptimizerRandomSearch$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.

Examples

```
search_space = domain = ps(x = p_dbl(lower = -1, upper = 1))

codomain = ps(y = p_dbl(tags = "minimize"))

objective_function = function(xs) {
  list(y = as.numeric(xs)^2)
}

objective = ObjectiveRFun$new(
 fun = objective_function,
 domain = domain,
 codomain = codomain)

instance = OptimInstanceSingleCrit$new(
 objective = objective,
 search_space = search_space,
 terminator = trm("evals", n_evals = 10))


optimizer = opt("random_search")

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

# returns best scoring evaluation
instance$result

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

---

mlr_terminators *Dictionary of Terminators*

Description

A simple mlr3misc::Dictionary storing objects of class Terminator. Each terminator has an associated help page, see `mlr_terminators_[id]`.

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

For a more convenient way to retrieve and construct terminator, see `trm()`/`trms()`.

Format

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

Methods

See mlr3misc::Dictionary.

See Also

Sugar functions: `trm()`, `trms()`

Other Terminator: `Terminator`, `mlr_terminators_clock_time`, `mlr_terminators_combo`, `mlr_terminators_evals`, `mlr_terminators_none`, `mlr_terminators_perf_reached`, `mlr_terminators_run_time`, `mlr_terminators_stagnatio`, `mlr_terminators_stagnation`

Examples

```
trm("evals", n_evals = 10)
```

---

mlr_terminators_clock_time

Terminator that stops according to the clock time

Description

Class to terminate the optimization after a fixed time point has been reached (as reported by `Sys.time()`).

Dictionary

This Terminator can be instantiated via the dictionary mlr_terminators or with the associated sugar function `trm()`:

```
mlr_terminators$get("clock_time")
trm("clock_time")
```

Parameters

`stop_time POSIXct(1)`
: Terminator stops after this point in time.

Super class

`bbotk::Terminator` -> `TerminatorClockTime`

Methods

Public methods:

- `TerminatorClockTime$new()`
- `TerminatorClockTime$is_terminated()`
- `TerminatorClockTime$clone()`

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

Usage:

```
TerminatorClockTime$new()
```

Method `is_terminated()`**:** Is `TRUE` iff the termination criterion is positive, and `FALSE` otherwise.

Usage:

```
TerminatorClockTime$is_terminated(archive)
```

Arguments:

`archive` (Archive).

Returns: `logical(1)`.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

See Also

Other Terminator: `Terminator`, `mlr_terminators_combo`, `mlr_terminators_evals`, `mlr_terminators_none`, `mlr_terminators_perf_reached`, `mlr_terminators_run_time`, `mlr_terminators_stagnation_batch`, `mlr_terminators_stagnation`, `mlr_terminators`

Examples

```
stop_time = as.POSIXct("2030-01-01 00:00:00")
trm("clock_time", stop_time = stop_time)
```

`mlr_terminators_combo` *Combine Terminators*

Description

This class takes multiple Terminators and terminates as soon as one or all of the included terminators are positive.

Dictionary

This Terminator can be instantiated via the dictionary mlr_terminators or with the associated sugar function `trm()`:

```
mlr_terminators$get("combo")
trm("combo")
```

Parameters

`any logical(1)`
: Terminate iff any included terminator is positive? (not all), default is `TRUE`.

Super class

`bbotk::Terminator` -> `TerminatorCombo`

Public fields

`terminators (list())`
: List of objects of class Terminator.

Methods

Public methods:

- `TerminatorCombo$new()`
- `TerminatorCombo$is_terminated()`
- `TerminatorCombo$print()`
- `TerminatorCombo$remaining_time()`
- `TerminatorCombo$status_long()`
- `TerminatorCombo$clone()`

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

Usage:

```
TerminatorCombo$new(terminators = list(TerminatorNone$new()))
```

Arguments:

`terminators (list())`
: List of objects of class Terminator.

Method `is_terminated()`: Is `TRUE` iff the termination criterion is positive, and `FALSE` otherwise.

Usage:

```
TerminatorCombo$is_terminated(archive)
```

Arguments:

`archive` (Archive).

Returns: `logical(1)`.

Method `print()`: Printer.

Usage:

```
TerminatorCombo$print(...)
```

Arguments:

`...` (ignored).

Method `remaining_time()`: Returns the remaining runtime in seconds. If `any = TRUE`, the remaining runtime is determined by the time-based terminator with the shortest time remaining. If non-time-based terminators are used and `any = FALSE`, the the remaining runtime is always `Inf`.

Usage:

```
TerminatorCombo$remaining_time(archive)
```

Arguments:

`archive` (Archive).

Returns: `integer(1)`.

Method `status_long()`: Returns `max_steps` and `current_steps` for each terminator.

Usage:

```
TerminatorCombo$status_long(archive)
```

Arguments:

`archive` (Archive).

Returns: data.table::data.table.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

See Also

Other Terminator: `Terminator`, `mlr_terminators_clock_time`, `mlr_terminators_evals`, `mlr_terminators_none`, `mlr_terminators_perf_reached`, `mlr_terminators_run_time`, `mlr_terminators_stagnation_batch`, `mlr_terminators_stagnation`, `mlr_terminators`

Examples

```
trm("combo",
  list(trm("clock_time", stop_time = Sys.time() + 60),
    trm("evals", n_evals = 10)), any = FALSE
)
```

`mlr_terminators_evals` *Terminator that stops after a number of evaluations*

Description

Class to terminate the optimization depending on the number of evaluations. An evaluation is defined by one resampling of a parameter value. The total number of evaluations B is defined as

$$B = \mathrm{n_e vals} + k * D$$

where D is the dimension of the search space.

Dictionary

This Terminator can be instantiated via the dictionary mlr_terminators or with the associated sugar function `trm()`:

```
mlr_terminators$get("evals")
trm("evals")
```

Parameters

`n_evals integer(1)`
: See formula above. Default is 100.

`k integer(1)`
: See formula above. Default is 0.

Super class

`bbotk::Terminator` -> `TerminatorEvals`

Methods

Public methods:

- `TerminatorEvals$new()`
- `TerminatorEvals$is_terminated()`
- `TerminatorEvals$clone()`

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

Usage:

```
TerminatorEvals$new()
```

Method `is_terminated()`**:** Is `TRUE` iff the termination criterion is positive, and `FALSE` otherwise.

Usage:

```
TerminatorEvals$is_terminated(archive)
```

Arguments:

`archive` (Archive).

Returns: `logical(1)`.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

See Also

Other Terminator: Terminator, mlr_terminators_clock_time, mlr_terminators_combo, mlr_terminators_none, mlr_terminators_perf_reached, mlr_terminators_run_time, mlr_terminators_stagnation_batch, mlr_terminators_stagnation, mlr_terminators

Examples

```
TerminatorEvals$new()

# 5 evaluations in total
trm("evals", n_evals = 5)

# 3 * [dimension of search space] evaluations in total
trm("evals", n_evals = 0, k = 3)

# (3 * [dimension of search space] + 1) evaluations in total
trm("evals", n_evals = 1, k = 3)
```

---

mlr_terminators_none *Terminator that never stops.*

Description

Mainly useful for optimization algorithms where the stopping is inherently controlled by the algorithm itself (e.g. OptimizerGridSearch).

Dictionary

This Terminator can be instantiated via the dictionary mlr_terminators or with the associated sugar function `trm()`:

```
mlr_terminators$get("none")
trm("none")
```

Super class

`bbotk::Terminator` -> `TerminatorNone`

Methods

Public methods:

- `TerminatorNone$new()`
- `TerminatorNone$is_terminated()`
- `TerminatorNone$clone()`

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

Usage:

```
TerminatorNone$new()
```

Method `is_terminated()`**:** Is `TRUE` iff the termination criterion is positive, and `FALSE` otherwise.

Usage:

```
TerminatorNone$is_terminated(archive)
```

Arguments:

`archive` (Archive).

Returns: `logical(1)`.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

See Also

Other Terminator: `Terminator`, `mlr_terminators_clock_time`, `mlr_terminators_combo`, `mlr_terminators_evals`, `mlr_terminators_perf_reached`, `mlr_terminators_run_time`, `mlr_terminators_stagnation_batch`, `mlr_terminators_stagnation`, `mlr_terminators`

`mlr_terminators_perf_reached` *Terminator that stops when a performance level has been reached*

Description

Class to terminate the optimization after a performance level has been hit.

Dictionary

This Terminator can be instantiated via the dictionary mlr_terminators or with the associated sugar function `trm()`:

```
mlr_terminators$get("perf_reached")
trm("perf_reached")
```

Parameters

`level numeric(1)`
: Performance level that needs to be reached, default is 0. Terminates if the performance exceeds (respective measure has to be maximized) or falls below (respective measure has to be minimized) this value.

Super class

`bbotk::Terminator` -> `TerminatorPerfReached`

Methods

Public methods:

- `TerminatorPerfReached$new()`
- `TerminatorPerfReached$is_terminated()`
- `TerminatorPerfReached$clone()`

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

Usage:

```
TerminatorPerfReached$new()
```

Method `is_terminated()`**:** Is `TRUE` iff the termination criterion is positive, and `FALSE` otherwise.

Usage:

```
TerminatorPerfReached$is_terminated(archive)
```

Arguments:

`archive` (Archive).

Returns: `logical(1)`.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

See Also

Other Terminator: `Terminator`, `mlr_terminators_clock_time`, `mlr_terminators_combo`, `mlr_terminators_evals`, `mlr_terminators_none`, `mlr_terminators_run_time`, `mlr_terminators_stagnation_batch`, `mlr_terminators_stagnation`, `mlr_terminators`

Examples

```
TerminatorPerfReached$new()
trm("perf_reached")
```

---

mlr_terminators_run_time

Terminator that stops according to the run time

Description

Class to terminate the optimization after the optimization process took a number of seconds on the clock.

Dictionary

This Terminator can be instantiated via the dictionary mlr_terminators or with the associated sugar function `trm()`:

```
mlr_terminators$get("run_time")
trm("run_time")
```

Parameters

`secs numeric(1)`
: Maximum allowed time, in seconds, default is 100.

Super class

`bbotk::Terminator` -> `TerminatorRunTime`

Methods

Public methods:

- TerminatorRunTime$new()
- TerminatorRunTime$is_terminated()
- TerminatorRunTime$clone()

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

Usage:

```
TerminatorRunTime$new()
```

Method `is_terminated()`**:** Is `TRUE` iff the termination criterion is positive, and `FALSE` otherwise.

Usage:

```
TerminatorRunTime$is_terminated(archive)
```

Arguments:

`archive` (Archive).

Returns: `logical(1)`.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Note

This terminator only works if `archive$start_time` is set. This is usually done by the Optimizer.

See Also

Other Terminator: Terminator, mlr_terminators_clock_time, mlr_terminators_combo, mlr_terminators_evals, mlr_terminators_none, mlr_terminators_perf_reached, mlr_terminators_stagnation_batch, mlr_terminators_stagnation, mlr_terminators

Examples

```
trm("run_time", secs = 1800)
```

`mlr_terminators_stagnation` *Terminator that stops when optimization does not improve*

Description

Class to terminate the optimization after the performance stagnates, i.e. does not improve more than `threshold` over the last `iters` iterations.

Dictionary

This Terminator can be instantiated via the dictionary mlr_terminators or with the associated sugar function `trm()`:

```
mlr_terminators$get("stagnation")
trm("stagnation")
```

Parameters

`iters integer(1)`
: Number of iterations to evaluate the performance improvement on, default is 10.

`threshold numeric(1)`
: If the improvement is less than `threshold`, optimization is stopped, default is `0`.

Super class

`bbotk::Terminator` -> `TerminatorStagnation`

Methods

Public methods:

- `TerminatorStagnation$new()`
- `TerminatorStagnation$is_terminated()`
- `TerminatorStagnation$clone()`

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

Usage:

```
TerminatorStagnation$new()
```

Method `is_terminated()`**:** Is `TRUE` iff the termination criterion is positive, and `FALSE` otherwise.

Usage:

```
TerminatorStagnation$is_terminated(archive)
```

Arguments:

`archive` (Archive).

Returns: `logical(1)`.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

See Also

Other Terminator: `Terminator`, `mlr_terminators_clock_time`, `mlr_terminators_combo`, `mlr_terminators_evals`, `mlr_terminators_none`, `mlr_terminators_perf_reached`, `mlr_terminators_run_time`, `mlr_terminators_stagnatio` `mlr_terminators`

Examples

```
TerminatorStagnation$new()
trm("stagnation", iters = 5, threshold = 1e-5)
```

`mlr_terminators_stagnation_batch`
Terminator that stops when optimization does not improve

Description

Class to terminate the optimization after the performance stagnates, i.e. does not improve more than `threshold` over the last `n` batches.

Dictionary

This Terminator can be instantiated via the dictionary mlr_terminators or with the associated sugar function `trm()`:

```
mlr_terminators$get("stagnation_batch")
trm("stagnation_batch")
```

Parameters

`n integer(1)`
: Number of batches to evaluate the performance improvement on, default is 1.

`threshold numeric(1)`
: If the improvement is less than `threshold`, optimization is stopped, default is `0`.

Super class

`bbotk::Terminator` -> `TerminatorStagnationBatch`

Methods

Public methods:

- `TerminatorStagnationBatch$new()`
- `TerminatorStagnationBatch$is_terminated()`
- `TerminatorStagnationBatch$clone()`

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

Usage:

```
TerminatorStagnationBatch$new()
```

Method `is_terminated()`**:** Is `TRUE` iff the termination criterion is positive, and `FALSE` otherwise.

Usage:

```
TerminatorStagnationBatch$is_terminated(archive)
```

Arguments:

`archive` (Archive).

Returns: `logical(1)`.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

See Also

Other Terminator: `Terminator`, `mlr_terminators_clock_time`, `mlr_terminators_combo`, `mlr_terminators_evals`, `mlr_terminators_none`, `mlr_terminators_perf_reached`, `mlr_terminators_run_time`, `mlr_terminators_stagnatio`
`mlr_terminators`

Examples

```
TerminatorStagnationBatch$new()
trm("stagnation_batch", n = 1, threshold = 1e-5)
```

`Objective` *Objective function with domain and co-domain*

Description

Describes a black-box objective function that maps an arbitrary domain to a numerical codomain.

Technical details

`Objective` objects can have the following properties: `"noisy"`, `"deterministic"`, `"single-crit"` and `"multi-crit"`.

Public fields

`id (character(1))`.

`properties (character())`.

`domain` (paradox::ParamSet)
Specifies domain of function, hence its input parameters, their types and ranges.

`codomain` (paradox::ParamSet)
Specifies codomain of function, hence its feasible values.

`constants` (paradox::ParamSet).
Changeable constants or parameters that are not subject to tuning can be stored and accessed here. Set constant values are passed to $.eval() and $.eval_many() as named arguments.

`check_values (logical(1))`

Active bindings

`xdim (integer(1))`
Dimension of domain.

`ydim (integer(1))`
Dimension of codomain.

Methods

Public methods:

- `Objective$new()`
- `Objective$format()`
- `Objective$print()`
- `Objective$eval()`
- `Objective$eval_many()`
- `Objective$eval_dt()`
- `Objective$clone()`

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

Usage:

```
Objective$new(
  id = "f",
  properties = character(),
  domain,
  codomain = ps(y = p_dbl(tags = "minimize")),
  constants = ps(),
  check_values = TRUE
)
```

Arguments:

`id` (`character(1)`).

`properties` (`character()`).

`domain` (paradox::ParamSet)
: Specifies domain of function. The paradox::ParamSet should describe all possible input parameters of the objective function. This includes their `id`, their types and the possible range.

`codomain` (paradox::ParamSet)
: Specifies codomain of function. Most importantly the tags of each output "Parameter" define whether it should be minimized or maximized. The default is to minimize each component.

`constants` (paradox::ParamSet)
: Changeable constants or parameters that are not subject to tuning can be stored and accessed here.

`check_values` (`logical(1)`)
: Should points before the evaluation and the results be checked for validity?

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

Usage:

```
Objective$format()
```

Returns: `character()`.

Method `print()`**:** Print method.

Usage:

```
Objective$print()
```

Returns: `character()`.

Method `eval()`**:** Evaluates a single input value on the objective function. If `check_values = TRUE`, the validity of the point as well as the validity of the result is checked.

Usage:

```
Objective$eval(xs)
```

Arguments:

`xs` (`list()`)
: A list that contains a single x value, e.g. `list(x1 = 1, x2 = 2)`.

Returns: `list()` that contains the result of the evaluation, e.g. `list(y = 1)`. The list can also contain additional *named* entries that will be stored in the archive if called through the OptimInstance. These extra entries are referred to as *extras*.

Method `eval_many()`**:** Evaluates multiple input values on the objective function. If `check_values = TRUE`, the validity of the points as well as the validity of the results are checked. *bbotk* does not take care of parallelization. If the function should make use of parallel computing, it has to be implemented by deriving from this class and overwriting this function.

Usage:

```
Objective$eval_many(xss)
```

Arguments:

`xss (list())`
A list of lists that contains multiple x values, e.g. `list(list(x1 = 1,x2 = 2),list(x1 = 3,x2 = 4))`.

Returns: data.table::data.table()] that contains one y-column for single-criteria functions and multiple y-columns for multi-criteria functions, e.g. `data.table(y = 1:2)` or `data.table(y1 = 1:2,y2 = 3:4)`. It may also contain additional columns that will be stored in the archive if called through the OptimInstance. These extra columns are referred to as *extras*.

Method `eval_dt()`**:** Evaluates multiple input values on the objective function

Usage:

```
Objective$eval_dt(xdt)
```

Arguments:

`xdt (data.table::data.table())`
Set of untransformed points / points from the *search space*. One point per row, e.g. `data.table(x1 = c(1,3),x2 = c(2,4))`. Column names have to match ids of the `search_space`. However, `xdt` can contain additional columns.

Returns: data.table::data.table()] that contains one y-column for single-criteria functions and multiple y-columns for multi-criteria functions, e.g. `data.table(y = 1:2)` or `data.table(y1 = 1:2,y2 = 3:4)`.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

`ObjectiveRFun` *Objective interface with custom R function*

Description

Objective interface where the user can pass a custom R function that expects a list as input.

Super class

`bbotk::Objective` -> `ObjectiveRFun`

Active bindings

`fun (function)`
Objective function.

Methods

Public methods:

- `ObjectiveRFun$new()`
- `ObjectiveRFun$eval()`
- `ObjectiveRFun$clone()`

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

Usage:

```
ObjectiveRFun$new(
  fun,
  domain,
  codomain = NULL,
  id = "function",
  properties = character(),
  constants = ps(),
  check_values = TRUE
)
```

Arguments:

`fun (function)`
R function that encodes objective and expects a list with the input for a single point (e.g. `list(x1 = 1, x2 = 2)`) and returns the result either as a numeric vector or a list (e.g. `list(y = 3)`).

`domain (paradox::ParamSet)`
Specifies domain of function. The paradox::ParamSet should describe all possible input parameters of the objective function. This includes their `id`, their types and the possible range.

`codomain (paradox::ParamSet)`
Specifies codomain of function. Most importantly the tags of each output "Parameter" define whether it should be minimized or maximized. The default is to minimize each component.

`id (character(1))`.

`properties (character())`.

`constants (paradox::ParamSet)`
Changeable constants or parameters that are not subject to tuning can be stored and accessed here.

`check_values (logical(1))`
Should points before the evaluation and the results be checked for validity?

Method `eval()`**:** Evaluates input value(s) on the objective function. Calls the R function supplied by the user.

Usage:

```
ObjectiveRFun$eval(xs)
```

Arguments:

`xs` Input values.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Examples

```
# define objective function
fun = function(xs) {
  - (xs[[1]] - 2)^2 - (xs[[2]] + 3)^2 + 10
}

# set domain
domain = ps(
  x1 = p_dbl(-10, 10),
  x2 = p_dbl(-5, 5)
)

# set codomain
codomain = ps(y = p_dbl(tags = "maximize"))

# create Objective object
obfun = ObjectiveRFun$new(
  fun = fun,
  domain = domain,
  codomain = codomain,
  properties = "deterministic"
)
```

ObjectiveRFunDt *Objective interface for basic R functions.*

Description

Objective interface where user can pass an R function that works on an `data.table()`.

Super class

`bbotk::Objective` -> `ObjectiveRFunDt`

Active bindings

`fun` (`function`)
Objective function.

Methods

Public methods:

- `ObjectiveRFunDt$new()`
- `ObjectiveRFunDt$eval_many()`
- `ObjectiveRFunDt$eval_dt()`
- `ObjectiveRFunDt$clone()`

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

Usage:

```
ObjectiveRFunDt$new(
  fun,
  domain,
  codomain = NULL,
  id = "function",
  properties = character(),
  constants = ps(),
  check_values = TRUE
)
```

Arguments:

`fun` (`function`)
: R function that encodes objective and expects an `data.table()` as input whereas each point is represented by one row.

`domain` (paradox::ParamSet)
: Specifies domain of function. The paradox::ParamSet should describe all possible input parameters of the objective function. This includes their `id`, their types and the possible range.

`codomain` (paradox::ParamSet)
: Specifies codomain of function. Most importantly the tags of each output "Parameter" define whether it should be minimized or maximized. The default is to minimize each component.

`id` (`character(1)`).

`properties` (`character()`).

`constants` (paradox::ParamSet)
: Changeable constants or parameters that are not subject to tuning can be stored and accessed here.

`check_values` (`logical(1)`)
: Should points before the evaluation and the results be checked for validity?

Method `eval_many()`**:** Evaluates multiple input values received as a list, converted to a `data.table()` on the objective function. Missing columns in xss are filled with `NA`s in `xdt`.

Usage:

```
ObjectiveRFunDt$eval_many(xss)
```

Arguments:

`xss` (`list()`)
: A list of lists that contains multiple x values, e.g. `list(list(x1 = 1, x2 = 2), list(x1 = 3, x2 = 4))`.

Returns: data.table::data.table() that contains one y-column for single-criteria functions and multiple y-columns for multi-criteria functions, e.g. `data.table(y = 1:2)` or `data.table(y1 = 1:2, y2 = 3:4)`.

Method `eval_dt()`**:** Evaluates multiple input values on the objective function supplied by the user.

Usage:

```
ObjectiveRFunDt$eval_dt(xdt)
```

Arguments:

`xdt` (data.table::data.table())
: Set of untransformed points / points from the *search space*. One point per row, e.g. `data.table(x1 = c(1,3), x2 = c(2,4))`. Column names have to match ids of the `search_space`. However, `xdt` can contain additional columns.

Returns: data.table::data.table()] that contains one y-column for single-criteria functions and multiple y-columns for multi-criteria functions, e.g. `data.table(y = 1:2)` or `data.table(y1 = 1:2, y2 = 3:4)`.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

`opt` *Syntactic Sugar Optimizer Construction*

Description

This function complements mlr_optimizers with functions in the spirit of `mlr_sugar` from **mlr3**.

Usage

```
opt(.key, ...)

opts(.keys, ...)
```

Arguments

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

Value

- Optimizer for `opt()`.
- list of Optimizer for `opts()`.

Examples

```
opt("random_search", batch_size = 10)
```

OptimInstance *Optimization Instance with budget and archive*

Description

Abstract base class.

Technical details

The Optimizer writes the final result to the `.result` field by using the $assign_result() method. `.result` stores a data.table::data.table consisting of x values in the *search space*, (transformed) x values in the *domain space* and y values in the *codomain space* of the Objective. The user can access the results with active bindings (see below).

Public fields

`objective` (Objective).

`search_space` (paradox::ParamSet).

`terminator` (Terminator).

`archive` (Archive).

`progressor` (`progressor()`)
Stores `progressor` function.

`objective_multiplicator` (`integer()`).

Active bindings

`result` (data.table::data.table)
Get result

`result_x_search_space` (data.table::data.table)
x part of the result in the *search space*.

`result_x_domain` (`list()`)
(transformed) x part of the result in the *domain space* of the objective.

`result_y` (`numeric()`)
Optimal outcome.

`is_terminated` (`logical(1)`).

Methods

Public methods:

- `OptimInstance$new()`
- `OptimInstance$format()`
- `OptimInstance$print()`
- `OptimInstance$eval_batch()`
- `OptimInstance$assign_result()`
- `OptimInstance$objective_function()`
- `OptimInstance$clear()`
- `OptimInstance$clone()`

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

Usage:

```
OptimInstance$new(
  objective,
  search_space = NULL,
  terminator,
  keep_evals = "all",
  check_values = TRUE
)
```

Arguments:

`objective` (Objective).

`search_space` (paradox::ParamSet)
Specifies the search space for the Optimizer. The paradox::ParamSet describes either a subset of the `domain` of the Objective or it describes a set of parameters together with a `trafo` function that transforms values from the search space to values of the domain. Depending on the context, this value defaults to the domain of the objective.

`terminator` (Terminator).

`keep_evals` (`character(1)`)
Keep `all` or only `best` evaluations in archive?

`check_values` (`logical(1)`)
Should x-values that are added to the archive be checked for validity? Search space that is logged into archive.

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

Usage:

```
OptimInstance$format()
```

Method `print()`**:** Printer.

Usage:

```
OptimInstance$print(...)
```

Arguments:

`...` (ignored).

Method `eval_batch()`**:** Evaluates all input values in `xdt` by calling the Objective. Applies possible transformations to the input values and writes the results to the Archive.
Before each batch-evaluation, the Terminator is checked, and if it is positive, an exception of class `terminated_error` is raised. This function should be internally called by the Optimizer.

Usage:

```
OptimInstance$eval_batch(xdt)
```

Arguments:

`xdt (data.table::data.table())`
x values as `data.table()` with one point per row. Contains the value in the *search space* of the OptimInstance object. Can contain additional columns for extra information.

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

Usage:

```
OptimInstance$assign_result(xdt, y)
```

Arguments:

`xdt (data.table::data.table())`
x values as `data.table()` with one row. Contains the value in the *search space* of the OptimInstance object. Can contain additional columns for extra information.

`y (numeric(1))`
Optimal outcome.

Method `objective_function()`**:** Evaluates (untransformed) points of only numeric values. Returns a numeric scalar for single-crit or a numeric vector for multi-crit. The return value(s) are negated if the measure is maximized. Internally, $eval_batch() is called with a single row. This function serves as a objective function for optimizers of numeric spaces - which should always be minimized.

Usage:

```
OptimInstance$objective_function(x)
```

Arguments:

`x (numeric())`
Untransformed points.

Returns: Objective value as `numeric(1)`, negated for maximization problems.

Method `clear()`**:** Reset terminator and clear all evaluation results from archive and results.

Usage:

```
OptimInstance$clear()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

`OptimInstanceMultiCrit` *Optimization Instance with budget and archive*

Description

Wraps a multi-criteria Objective function with extra services for convenient evaluation. Inherits from OptimInstance.

- Automatic storing of results in an Archive after evaluation.
- Automatic checking for termination. Evaluations of design points are performed in batches. Before a batch is evaluated, the 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.

Super class

`bbotk::OptimInstance` -> `OptimInstanceMultiCrit`

Active bindings

`result_x_domain (list())`
(transformed) x part of the result in the *domain space* of the objective.

`result_y (numeric(1))`
Optimal outcome.

Methods

Public methods:

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

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

Usage:

```
OptimInstanceMultiCrit$new(
  objective,
  search_space = NULL,
  terminator,
  keep_evals = "all",
  check_values = TRUE
)
```

Arguments:

`objective` (Objective).

`search_space` (paradox::ParamSet)
: Specifies the search space for the Optimizer. The paradox::ParamSet describes either a subset of the `domain` of the Objective or it describes a set of parameters together with a `trafo` function that transforms values from the search space to values of the domain. Depending on the context, this value defaults to the domain of the objective.

`terminator` (Terminator)
: Multi-criteria terminator.

`keep_evals` (`character(1)`)
: Keep `all` or only `best` evaluations in archive?

`check_values` (`logical(1)`)
: Should x-values that are added to the archive be checked for validity? Search space that is logged into archive.

Method `assign_result()`**:** The Optimizer object writes the best found points and estimated performance values here (probably the Pareto set / front). For internal use.

Usage:

```
OptimInstanceMultiCrit$assign_result(xdt, ydt)
```

Arguments:

`xdt` (`data.table::data.table()`)
: Set of untransformed points / points from the *search space*. One point per row, e.g. `data.table(x1 = c(1,3),x2 = c(2,4))`. Column names have to match ids of the `search_space`. However, `xdt` can contain additional columns.

`ydt` (`numeric(1)`)
: Optimal outcomes, e.g. the Pareto front.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

`OptimInstanceSingleCrit` *Optimization Instance with budget and archive*

Description

Wraps a single-criteria Objective function with extra services for convenient evaluation. Inherits from OptimInstance.

- Automatic storing of results in an Archive after evaluation.
- Automatic checking for termination. Evaluations of design points are performed in batches. Before a batch is evaluated, the 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.

Super class

`bbotk::OptimInstance` -> `OptimInstanceSingleCrit`

Methods

Public methods:

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

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

Usage:

```
OptimInstanceSingleCrit$new(
  objective,
  search_space = NULL,
  terminator,
  keep_evals = "all",
  check_values = TRUE
)
```

Arguments:

`objective` (Objective).

`search_space` (paradox::ParamSet)
: Specifies the search space for the Optimizer. The paradox::ParamSet describes either a subset of the `domain` of the Objective or it describes a set of parameters together with a `trafo` function that transforms values from the search space to values of the domain. Depending on the context, this value defaults to the domain of the objective.

`terminator` (Terminator).

`keep_evals` (`character(1)`)
: Keep `all` or only `best` evaluations in archive?

`check_values` (`logical(1)`)
: Should x-values that are added to the archive be checked for validity? Search space that is logged into archive.

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

Usage:

```
OptimInstanceSingleCrit$assign_result(xdt, y)
```

Arguments:

`xdt` (`data.table::data.table()`)
: Set of untransformed points / points from the *search space*. One point per row, e.g. `data.table(x1 = c(1,3),x2 = c(2,4))`. Column names have to match ids of the `search_space`. However, `xdt` can contain additional columns.

`y` (`numeric(1)`)
: Optimal outcome.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

`Optimizer` *Optimizer*

Description

Abstract `Optimizer` class that implements the base functionality each `Optimizer` subclass must provide. A `Optimizer` object describes the optimization strategy.

A `Optimizer` object must write its result to the $assign_result() method of the OptimInstance at the end in order to store the best point and its estimated performance vector.

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")`.

Public fields

`param_classes` (`character()`).

`properties` (`character()`).

`packages` (`character()`).

Active bindings

`param_set` (paradox::ParamSet).

Methods

Public methods:

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

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

Usage:

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

Arguments:

param_set (paradox::ParamSet).

param_classes (character()).

properties (character()).

packages (character()).

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

Usage:

```
Optimizer$format()
```

Method `print()`**:** Print method.

Usage:

```
Optimizer$print()
```

Returns: (character()).

Method `optimize()`**:** Performs the optimization and writes optimization result into OptimInstance. The optimization result is returned but the complete optimization path is stored in Archive of OptimInstance.

Usage:

```
Optimizer$optimize(inst)
```

Arguments:

inst (OptimInstance).

Returns: data.table::data.table.

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

Usage:

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

Arguments:

deep Whether to make a deep clone.

`Progressor` *Progressor*

Description

Wraps `progressr::progressor()` function and stores current progress.

Public fields

progressor (progressr::progressor()).

max_steps (integer(1)).

current_steps (integer(1)).

unit (character(1)).

Methods

Public methods:

- `Progressor$new()`
- `Progressor$update()`
- `Progressor$clone()`

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

Usage:

```
Progressor$new(progressor, unit)
```

Arguments:

`progressor` (`progressr::progressor()`)
Progressor function.

`unit` (`character(1)`)
Unit of progress.

Method `update()`**:** Updates `progressr::progressor()` with current steps.

Usage:

```
Progressor$update(terminator, archive)
```

Arguments:

`terminator` (Terminator).

`archive` (Archive).

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

`Terminator` *Abstract Terminator Class*

Description

Abstract `Terminator` class that implements the base functionality each terminator must provide. A terminator is an object that determines when to stop the optimization.

Termination of optimization works as follows:

- Evaluations in a instance are performed in batches.
- Before each batch evaluation, the Terminator is checked, and if it is positive, we stop.
- The optimization algorithm itself might decide not to produce any more points, or even might decide to do a smaller batch in its last evaluation.

Therefore the following note seems in order: While it is definitely possible to execute a fine-grained control for termination, and for many optimization algorithms we can specify exactly when to stop, it might happen that too few or even too many evaluations are performed, especially if multiple points are evaluated in a single batch (c.f. batch size parameter of many optimization algorithms). So it is advised to check the size of the returned archive, in particular if you are benchmarking multiple optimization algorithms.

Technical details

`Terminator` subclasses can overwrite `.status()` to support progress bars via the package **progressr**. The method must return the maximum number of steps (`max_steps`) and the currently achieved number of steps (`current_steps`) as a named integer vector.

Public fields

`param_set` paradox::ParamSet
: Set of control parameters for terminator.

`properties` (`character()`)
: Set of properties.

`unit` (`character()`)
: Unit of steps.

Methods

Public methods:

- `Terminator$new()`
- `Terminator$format()`
- `Terminator$print()`
- `Terminator$status()`
- `Terminator$remaining_time()`
- `Terminator$clone()`

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

Usage:

```
Terminator$new(param_set = ps(), properties = character())
```

Arguments:

`param_set` (paradox::ParamSet)
: Set of control parameters for terminator.

`properties` (`character()`)
: Set of properties.

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

Usage:

```
Terminator$format(with_params = FALSE)
```

Arguments:

`with_params (logical(1))`
Add parameter values to format string.

Method `print()`**:** Printer.

Usage:

```
Terminator$print(...)
```

Arguments:

`...` (ignored).

Method `status()`**:** Returns how many progression steps are made (`current_steps`) and the amount steps needed for termination (`max_steps`).

Usage:

```
Terminator$status(archive)
```

Arguments:

`archive` (Archive).

Returns: named `integer(2)`.

Method `remaining_time()`**:** Returns remaining runtime in seconds. If the terminator is not time-based, the reaming runtime is `Inf`.

Usage:

```
Terminator$remaining_time(archive)
```

Arguments:

`archive` (Archive).

Returns: `integer(1)`.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

See Also

Other Terminator: `mlr_terminators_clock_time`, `mlr_terminators_combo`, `mlr_terminators_evals`, `mlr_terminators_none`, `mlr_terminators_perf_reached`, `mlr_terminators_run_time`, `mlr_terminators_stagnatio` `mlr_terminators_stagnation`, `mlr_terminators`

`trm` *Syntactic Sugar Terminator Construction*

Description

This function complements mlr_terminators with functions in the spirit of `mlr_sugar` from **mlr3**.

Usage

```
trm(.key, ...)

trms(.keys, ...)
```

Arguments

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

Value

- Terminator for `trm()`.
- list of Terminator for `trms()`.

Examples

```
trm("evals", n_evals = 10)
```

Index