

Package ‘mlr3mbo’

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Type Package

Title Flexible Bayesian Optimization

Version 0.1.2

Description A modern and flexible approach to Bayesian Optimization / Model Based Optimization building on the 'bbotk' package. 'mlr3mbo' is a toolbox providing both ready-to-use optimization algorithms as well as their fundamental building blocks allowing for straightforward implementation of custom algorithms. Single- and multi-objective optimization is supported as well as mixed continuous, categorical and conditional search spaces. Moreover, using 'mlr3mbo' for hyperparameter optimization of machine learning models within the 'mlr3' ecosystem is straightforward via 'mlr3tuning'. Examples of ready-to-use optimization algorithms include Efficient Global Optimization by Jones et al. (1998) <doi:10.1023/A:1008306431147>, ParEGO by Knowles (2006) <doi:10.1109/TEVC.2005.851274> and SMS-EGO by Ponweiser et al. (2008) <doi:10.1007/978-3-540-87700-4_78>.

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 'AcqFunctionMean.R' 'AcqFunctionPI.R' 'AcqFunctionSmsEgo.R'
 'AcqOptimizer.R' 'aaa.R' 'OptimizerMbo.R' 'Surrogate.R'
 'SurrogateLearner.R' 'SurrogateLearnerCollection.R'
 'TunerMbo.R' 'mlr_loop_functions.R' 'bayesopt_ego.R'
 'bayesopt_mpcl.R' 'bayesopt_parego.R' 'bayesopt_smsego.R'
 'bibentries.R' 'helper.R' 'loop_function.R' 'mbo_defaults.R'
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mlr3mbo-package

mlr3mbo: Flexible Bayesian Optimization

Description

A modern and flexible approach to Bayesian Optimization / Model Based Optimization building on the 'bbotk' package. 'mlr3mbo' is a toolbox providing both ready-to-use optimization algorithms as well as their fundamental building blocks allowing for straightforward implementation of custom algorithms. Single- and multi-objective optimization is supported as well as mixed continuous, categorical and conditional search spaces. Moreover, using 'mlr3mbo' for hyperparameter optimization of machine learning models within the 'mlr3' ecosystem is straightforward via 'mlr3tuning'. Examples of ready-to-use optimization algorithms include Efficient Global Optimization by Jones et al. (1998) [doi:10.1023/A:1008306431147](https://doi.org/10.1023/A:1008306431147), ParEGO by Knowles (2006) [doi:10.1109/TEVC.2005.851274](https://doi.org/10.1109/TEVC.2005.851274) and SMS-EGO by Ponweiser et al. (2008) [doi:10.1007/9783540-877004_78](https://doi.org/10.1007/9783540-877004_78).

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See Also

Useful links:

- <https://mlr3mbo.mlr-org.com>
- <https://github.com/mlr-org/mlr3mbo>
- Report bugs at <https://github.com/mlr-org/mlr3mbo/issues>

acqf

Syntactic Sugar Acquisition Function Construction

Description

This function complements [mlr_acqfunctions](#) with functions in the spirit of `mlr_sugar` from **mlr3**.

Usage

```
acqf(.key, ...)
```

Arguments

<code>.key</code>	(character(1)) Key passed to the respective dictionary to retrieve the object.
<code>...</code>	(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.

Value

[AcqFunction](#)

Examples

```
acqf("ei")
```

AcqFunction

*Acquisition Function Base Class***Description**

Abstract acquisition function class.

Based on the predictions of a [Surrogate](#), the acquisition function encodes the preference to evaluate a new point.

Super class

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

Active bindings

direction ("same" | "minimize" | "maximize")

Optimization direction of the acquisition function relative to the direction of the objective function of the [bbotk::OptimInstance](#). Must be "same", "minimize", or "maximize".

surrogate_max_to_min (-1 | 1)

Multiplicative factor to correct for minimization or maximization of the acquisition function.

label (character(1))

Label for this object.

man (character(1))

String in the format [pkg]::[topic] pointing to a manual page for this object.

archive ([bbotk::Archive](#))

Points to the [bbotk::Archive](#) of the surrogate.

fun (function)

Pointing to the private acquisition function to be implemented by subclasses.

surrogate ([Surrogate](#))

Surrogate.

requires_predict_type_se (logical(1))

Whether the acquisition function requires the surrogate to have "se" as \$predict_type.

Methods**Public methods:**

- [AcqFunction\\$new\(\)](#)
- [AcqFunction\\$update\(\)](#)
- [AcqFunction\\$eval_many\(\)](#)
- [AcqFunction\\$eval_dt\(\)](#)
- [AcqFunction\\$clone\(\)](#)

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

Note that the surrogate can be initialized lazy and can later be set via the active binding \$surrogate.

Usage:

```
AcqFunction$new(
  id,
  constants = ParamSet$new(),
  surrogate,
  requires_predict_type_se,
  direction,
  label = NA_character_,
  man = NA_character_
)
```

Arguments:

`id` (character(1)).

`constants` ([paradox::ParamSet](#)). Changeable constants or parameters.

`surrogate` (NULL | [Surrogate](#)). Surrogate whose predictions are used in the acquisition function.

`requires_predict_type_se` (logical(1))

Whether the acquisition function requires the surrogate to have "se" as `$predict_type`.

`direction` ("same" | "minimize" | "maximize"). Optimization direction of the acquisition function relative to the direction of the objective function of the [bbotk::OptimInstance](#). Must be "same", "minimize", or "maximize".

`label` (character(1))

Label for this object.

`man` (character(1))

String in the format `[pkg]::[topic]` pointing to a manual page for this object.

Method `update()`: Update the acquisition function.

Can be implemented by subclasses.

Usage:

```
AcqFunction$update()
```

Method `eval_many()`: Evaluates multiple input values on the objective function.

Usage:

```
AcqFunction$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-objective functions and multiple y-columns for multi-objective 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

Usage:

```
AcqFunction$eval_dt(xdt)
```

Arguments:

xdt ([data.table::data.table\(\)](#))

One point per row, e.g. `data.table(x1 = c(1, 3), x2 = c(2, 4))`.

Returns: `data.table::data.table()` that contains one y-column for single-objective functions and multiple y-columns for multi-objective 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:

`AcqFunction$clone(deep = FALSE)`

Arguments:

`deep` Whether to make a deep clone.

See Also

Other Acquisition Function: [mlr_acqfunctions_aei](#), [mlr_acqfunctions_cb](#), [mlr_acqfunctions_eips](#), [mlr_acqfunctions_ei](#), [mlr_acqfunctions_mean](#), [mlr_acqfunctions_pi](#), [mlr_acqfunctions_smsego](#), [mlr_acqfunctions](#)

acqo

Syntactic Sugar Acquisition Function Optimizer Construction

Description

This function allows to construct an [AcqOptimizer](#) in the spirit of `mlr_sugar` from **mlr3**.

Usage

`acqo(optimizer, terminator, acq_function = NULL, ...)`

Arguments

<code>optimizer</code>	(bbotk::Optimizer) bbotk::Optimizer that is to be used.
<code>terminator</code>	(bbotk::Terminator) bbotk::Terminator that is to be used.
<code>acq_function</code>	(NULL AcqFunction) AcqFunction that is to be used. Can also be NULL.
<code>...</code>	(named <code>list()</code>) Named arguments passed to the constructor, to be set as parameters in the paradox::ParamSet .

Value

[AcqOptimizer](#)

Examples

```
library(bbotk)
acqo(opt("random_search"), trm("evals"), catch_errors = FALSE)
```

AcqOptimizer

Acquisition Function Optimizer

Description

Optimizer for [AcqFunctions](#) which performs the infill optimization. Wraps an [bbotk::Optimizer](#) and [bbotk::Terminator](#).

Parameters

`logging_level` `character(1)`
 Logging level during the infill optimization. Can be "fatal", "error", "warn", "info", "debug" or "trace". Default is "warn", i.e., only warnings are logged.

`warmstart` `logical(1)`
 Should the infill optimization be warm-started by evaluating the best point(s) present in the [bbotk::Archive](#) of the actual [bbotk::OptimInstance](#)? This is sensible when using a population based infill optimizer, e.g., local search or mutation. Default is FALSE.

`warmstart_size` `integer(1) | "all"`
 Number of best points selected from the [bbotk::Archive](#) that are to be used for warm starting. Can also be "all" to use all available points. Only relevant if `warmstart = TRUE`. Default is 1.

`skip_already_evaluated` `logical(1)`
 It can happen that the candidate resulting of the infill optimization was already evaluated in a previous iteration. Should this candidate proposal be ignored and the next best point be selected as a candidate? Default is TRUE.

`catch_errors` `logical(1)`
 Should errors during the infill optimization be caught and propagated to the `loop_function` which can then handle the failed infill optimization appropriately by, e.g., proposing a randomly sampled point for evaluation? Default is TRUE.

Public fields

`optimizer` ([bbotk::Optimizer](#)).

`terminator` ([bbotk::Terminator](#)).

`acq_function` ([AcqFunction](#)).

Active bindings

`print_id` (`character`)
 Id used when printing.

`param_set` ([paradox::ParamSet](#))
 Set of hyperparameters.

Methods**Public methods:**

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

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

Usage:

```
AcqOptimizer$new(optimizer, terminator, acq_function = NULL)
```

Arguments:

`optimizer` ([bbotk::Optimizer](#)).

`terminator` ([bbotk::Terminator](#)).

`acq_function` (NULL | [AcqFunction](#)).

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

Usage:

```
AcqOptimizer$format()
```

Method `print()`: Print method.

Usage:

```
AcqOptimizer$print()
```

Returns: (`character()`).

Method `optimize()`: Optimize the acquisition function.

Usage:

```
AcqOptimizer$optimize()
```

Returns: [data.table::data.table\(\)](#) with 1 row per optimum and x as columns.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

default_acqfun	<i>Default Acquisition Function</i>
----------------	-------------------------------------

Description

Chooses a default acquisition function, i.e. the criterion used to propose future points. For single-objective optimization, defaults to [mlr_acqfunctions_ei](#). For multi-objective optimization, defaults to [mlr_acqfunctions_smsego](#).

Usage

```
default_acqfun(instance)
```

Arguments

instance ([bbotk::OptimInstance](#)).

Value

[AcqFunction](#)

See Also

Other mbo_defaults: [default_acqopt\(\)](#), [default_loopfun\(\)](#), [default_surrogate\(\)](#), [mbo_defaults](#)

default_acqopt	<i>Default Acquisition Function Optimizer</i>
----------------	---

Description

Chooses a default acquisition function optimizer. Defaults to wrapping [bbotk::OptimizerRandomSearch](#) allowing 10000 function evaluations (with a batch size of 1000) via a [bbotk::TerminatorEvals](#).

Usage

```
default_acqopt(acq_function)
```

Arguments

acq_function ([AcqFunction](#)).

Value

[AcqOptimizer](#)

See Also

Other mbo_defaults: [default_acqfun\(\)](#), [default_loopfun\(\)](#), [default_surrogate\(\)](#), [mbo_defaults](#)

default_loopfun	<i>Default Loop Function</i>
-----------------	------------------------------

Description

Chooses a default [loop_function](#), i.e. the Bayesian Optimization flavor to be used for optimization. For single-objective optimization, defaults to [bayesopt_ego](#). For multi-objective optimization, defaults to [bayesopt_smsego](#).

Usage

```
default_loopfun(instance)
```

Arguments

instance ([bbotk::OptimInstance](#))
An object that inherits from [bbotk::OptimInstance](#).

Value

[loop_function](#)

See Also

Other mbo_defaults: [default_acqfun\(\)](#), [default_acqopt\(\)](#), [default_surrogate\(\)](#), [mbo_defaults](#)

default_surrogate	<i>Default Surrogate</i>
-------------------	--------------------------

Description

This is a helper function that generates a default [Surrogate](#) based on properties of the [bbotk::OptimInstance](#). For numeric-only (including integers) parameter spaces without any dependencies:

- A Kriging model `"regr.km"` with kernel `"matern3_2"` is created.
- If the objective function is deterministic we add a small nugget effect ($10^{-8} \cdot \text{Var}(y)$, y is vector of observed outcomes in current design) to increase numerical stability to hopefully prevent crashes of **DiceKriging**. Whether the objective function is deterministic can be observed from the objective function's properties.
- If the objective function is noisy the nugget effect will be estimated with `nugget.estim = TRUE`.
- Also `jitter` is set to `TRUE` to circumvent a problem with **DiceKriging** where already trained input values produce the exact trained output. Whether the objective function is noisy can be observed from the objective functions properties.

- Instead of the default "BFGS" optimization method we use rgenoud ("gen"), which is a hybrid algorithm, to combine global search based on genetic algorithms and local search based on gradients. This may improve the model fit and will less frequently produce a constant surrogate model.

For mixed numeric-categorical parameter spaces, or spaces with conditional parameters:

- A ranger regression forest `"regr.ranger"` with 500 trees is created.
- The standard error of a prediction (if required by the infill criterion) is estimated via jackknife. This is the `se.method = "jack"` option of the `"regr.ranger"` learner (default).

In any case, learners are encapsulated using `"evaluate"`, and a fallback learner is set, in cases where the surrogate learner errors. Currently, the following learner is used as a fallback: `lrn("regr.ranger", num.trees = 20L, keep.inbag = TRUE, se.method = "jack")`.

If additionally dependencies are present in the parameter space, inactive conditional parameters are represented by missing NA values in the training design data. We simply handle those with an imputation method, added to the ranger random forest, more concretely we use `po("imputesample")` (for logicals) and `po("imputeoor")` (for anything else) from package **mlr3pipelines**. Characters are always encoded as factors via `po("colapply")`. Out of range imputation makes sense for tree-based methods and is usually hard to beat, see Ding et al. (2010). In the case of dependencies, the following learner is used as a fallback: `lrn("regr.featureless")`.

If the instance is of class `bbotk::OptimInstanceSingleCrit` the learner is wrapped as a [SurrogateLearner](#).

If the instance is of class `bbotk::OptimInstanceMultiCrit` deep clones of the learner are wrapped as a [SurrogateLearnerCollection](#).

Usage

```
default_surrogate(instance, learner = NULL, n_learner = NULL)
```

Arguments

instance	(<code>bbotk::OptimInstance</code>) An object that inherits from <code>bbotk::OptimInstance</code> .
learner	(NULL <code>mlr3::Learner</code>).
n_learner	(NULL <code>integer(1)</code>).

Value

[Surrogate](#)

References

- Ding, Yufeng, Simonoff, S J (2010). "An Investigation of Missing Data Methods for Classification Trees Applied to Binary Response Data." *Journal of Machine Learning Research*, **11**(1), 131–170.

See Also

Other `mbo_defaults`: [default_acqfun\(\)](#), [default_acqopt\(\)](#), [default_loopfun\(\)](#), [mbo_defaults](#)

loop_function	<i>Loop Functions for Bayesian Optimization</i>
---------------	---

Description

Loop functions determine the behavior of the Bayesian Optimization algorithm on a global level. For an overview of readily available loop functions, see `as.data.table(mlr_loop_functions)`.

In general, a loop function is simply a decorated member of the S3 class `loop_function`. Attributes must include: `id` (id of the loop function), `label` (brief description), `instance` ("single-crit" and or "multi-crit"), and `man` (link to the manual page).

As an example, see, e.g., [bayesopt_ego](#).

See Also

Other Loop Function: [mlr_loop_functions_ego](#), [mlr_loop_functions_mpcl](#), [mlr_loop_functions_parego](#), [mlr_loop_functions_smsego](#), [mlr_loop_functions](#)

mbo_defaults	<i>Defaults for OptimizerMbo</i>
--------------	----------------------------------

Description

The following defaults are set for `OptimizerMbo` during optimization if the respective fields are not set during initialization.

- Optimization Loop: [default_loopfun](#)
- Surrogate: [default_surrogate](#)
- Acquisition Function: [default_acqfun](#)
- Acqfun Optimizer: [default_acqopt](#)

See Also

Other `mbo_defaults`: [default_acqfun\(\)](#), [default_acqopt\(\)](#), [default_loopfun\(\)](#), [default_surrogate\(\)](#)

mlr_acqfunctions *Dictionary of Acquisition Functions*

Description

A simple `mlr3misc::Dictionary` storing objects of class `AcqFunction`. Each acquisition function has an associated help page, see `mlr_acqfunctions_[id]`.

For a more convenient way to retrieve and construct an acquisition function, see `acqf()`.

Format

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

Methods

See `mlr3misc::Dictionary`.

See Also

Sugar function: `acqf()`

Other Dictionary: `mlr_loop_functions`

Other Acquisition Function: `AcqFunction`, `mlr_acqfunctions_aei`, `mlr_acqfunctions_cb`, `mlr_acqfunctions_eips`, `mlr_acqfunctions_ei`, `mlr_acqfunctions_mean`, `mlr_acqfunctions_pi`, `mlr_acqfunctions_smsego`

Examples

```
as.data.table(mlr_acqfunctions)
acqf("ei")
```

mlr_acqfunctions_aei *Acquisition Function Augmented Expected Improvement*

Description

Augmented Expected Improvement. Useful when working with noisy objectives. Currently only works correctly with `"regr.km"` as surrogate model and `nugget.estim = TRUE` or given.

Dictionary

This `AcqFunction` can be instantiated via the dictionary `mlr_acqfunctions` or with the associated sugar function `acqf()`:

```
mlr_acqfunctions$get("aei")
acqf("aei")
```

Parameters

- "c" (numeric(1))
Constant c as used in Formula (14) of Huang (2012) to reflect the degree of risk aversion. Defaults to 1.

Super classes

`bbotk::Objective` -> `mlr3mbo::AcqFunction` -> `AcqFunctionAEI`

Public fields

`y_effective_best` (numeric(1))
Best effective objective value observed so far. In the case of maximization, this already includes the necessary change of sign.

`noise_var` (numeric(1))
Estimate of the variance of the noise. This corresponds to the nugget estimate when using a `mlr3learners` as surrogate model.

Methods**Public methods:**

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

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

Usage:

```
AcqFunctionAEI$new(surrogate = NULL, c = 1)
```

Arguments:

`surrogate` (NULL | `SurrogateLearner`).

`c` (numeric(1)).

Method `update()`: Updates acquisition function and sets `y_effective_best` and `noise_var`.

Usage:

```
AcqFunctionAEI$update()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

References

- Huang D, Allen TT, Notz WI, Zheng N (2012). "Erratum To: Global Optimization of Stochastic Black-box Systems via Sequential Kriging Meta-Models." *Journal of Global Optimization*, **54**(2), 431–431.

See Also

Other Acquisition Function: [AcqFunction](#), [mlr_acqfunctions_cb](#), [mlr_acqfunctions_eips](#), [mlr_acqfunctions_ei](#), [mlr_acqfunctions_mean](#), [mlr_acqfunctions_pi](#), [mlr_acqfunctions_smsego](#), [mlr_acqfunctions](#)

Examples

```

if (requireNamespace("mlr3learners") &
    requireNamespace("DiceKriging") &
    requireNamespace("rgenoud")) {
  library(bbotk)
  library(paradox)
  library(mlr3learners)
  library(data.table)

  set.seed(2906)
  fun = function(xs) {
    list(y = xs$x ^ 2 + rnorm(length(xs$x), mean = 0, sd = 1))
  }
  domain = ps(x = p_dbl(lower = -10, upper = 10))
  codomain = ps(y = p_dbl(tags = "minimize"))
  objective = ObjectiveRfun$new(fun = fun,
    domain = domain,
    codomain = codomain,
    properties = "noisy")

  instance = OptimInstanceSingleCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))

  instance$eval_batch(data.table(x = c(-6, -5, 3, 9)))

  learner = lrn("regr.km",
    covtype = "matern3_2",
    optim.method = "gen",
    nugget.estim = TRUE,
    jitter = 1e-12,
    control = list(trace = FALSE))

  surrogate = srlrn(learner, archive = instance$archive)

  acq_function = acqf("aei", surrogate = surrogate)

  acq_function$surrogate$update()
  acq_function$update()
  acq_function$eval_dt(data.table(x = c(-1, 0, 1)))
}

```

mlr_acqfunctions_cb *Acquisition Function Confidence Bound*

Description

Lower / Upper Confidence Bound.

Dictionary

This [AcqFunction](#) can be instantiated via the [dictionary mlr_acqfunctions](#) or with the associated sugar function `acqf()`:

```
mlr_acqfunctions$get("cb")
acqf("cb")
```

Parameters

- "lambda" (numeric(1))
λ value used for the confidence bound. Defaults to 2.

Super classes

[bbotk::Objective](#) -> [mlr3mbo::AcqFunction](#) -> [AcqFunctionCB](#)

Methods

Public methods:

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

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

Usage:

```
AcqFunctionCB$new(surrogate = NULL, lambda = 2)
```

Arguments:

surrogate (NULL | [SurrogateLearner](#)).

lambda (numeric(1)).

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

Usage:

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

Arguments:

deep Whether to make a deep clone.

References

- Snoek, Jasper, Larochelle, Hugo, Adams, P R (2012). “Practical Bayesian Optimization of Machine Learning Algorithms.” In Pereira F, Burges CJC, Bottou L, Weinberger KQ (eds.), *Advances in Neural Information Processing Systems*, volume 25, 2951–2959.

See Also

Other Acquisition Function: [AcqFunction](#), [mlr_acqfunctions_wei](#), [mlr_acqfunctions_eips](#), [mlr_acqfunctions_ei](#), [mlr_acqfunctions_mean](#), [mlr_acqfunctions_pi](#), [mlr_acqfunctions_smsego](#), [mlr_acqfunctions](#)

Examples

```
if (requireNamespace("mlr3learners") &
    requireNamespace("DiceKriging") &
    requireNamespace("rgenoud")) {
  library(bbotk)
  library(paradox)
  library(mlr3learners)
  library(data.table)

  fun = function(xs) {
    list(y = xs$x ^ 2)
  }
  domain = ps(x = p_dbl(lower = -10, upper = 10))
  codomain = ps(y = p_dbl(tags = "minimize"))
  objective = ObjectiveRFun$new(fun = fun, domain = domain, codomain = codomain)

  instance = OptimInstanceSingleCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))

  instance$eval_batch(data.table(x = c(-6, -5, 3, 9)))

  learner = lrn("regr.km",
    covtype = "matern3_2",
    optim.method = "gen",
    nugget.stability = 10^-8,
    control = list(trace = FALSE))

  surrogate = srlrn(learner, archive = instance$archive)

  acq_function = acqf("cb", surrogate = surrogate, lambda = 3)

  acq_function$surrogate$update()
  acq_function$eval_dt(data.table(x = c(-1, 0, 1)))
}
```

mlr_acqfunctions_ei *Acquisition Function Expected Improvement*

Description

Expected Improvement.

Dictionary

This [AcqFunction](#) can be instantiated via the [dictionary mlr_acqfunctions](#) or with the associated sugar function [acqf\(\)](#):

```
mlr_acqfunctions$get("ei")
acqf("ei")
```

Super classes

[bbotk::Objective](#) -> [mlr3mbo::AcqFunction](#) -> [AcqFunctionEI](#)

Public fields

`y_best` (numeric(1))

Best objective function value observed so far. In the case of maximization, this already includes the necessary change of sign.

Methods

Public methods:

- [AcqFunctionEI\\$new\(\)](#)
- [AcqFunctionEI\\$update\(\)](#)
- [AcqFunctionEI\\$clone\(\)](#)

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

Usage:

```
AcqFunctionEI$new(surrogate = NULL)
```

Arguments:

surrogate (NULL | [SurrogateLearner](#)).

Method `update()`: Updates acquisition function and sets `y_best`.

Usage:

```
AcqFunctionEI$update()
```

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

Usage:

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

Arguments:

deep Whether to make a deep clone.

References

- Jones, R. D, Schonlau, Matthias, Welch, J. W (1998). “Efficient Global Optimization of Expensive Black-Box Functions.” *Journal of Global optimization*, **13**(4), 455–492.

See Also

Other Acquisition Function: [AcqFunction](#), [mlr_acqfunctions_aei](#), [mlr_acqfunctions_cb](#), [mlr_acqfunctions_eips](#), [mlr_acqfunctions_mean](#), [mlr_acqfunctions_pi](#), [mlr_acqfunctions_smsego](#), [mlr_acqfunctions](#)

Examples

```
if (requireNamespace("mlr3learners") &
    requireNamespace("DiceKriging") &
    requireNamespace("rgenoud")) {
  library(bbotk)
  library(paradox)
  library(mlr3learners)
  library(data.table)

  fun = function(xs) {
    list(y = xs$x ^ 2)
  }
  domain = ps(x = p_dbl(lower = -10, upper = 10))
  codomain = ps(y = p_dbl(tags = "minimize"))
  objective = ObjectiveRFun$new(fun = fun, domain = domain, codomain = codomain)

  instance = OptimInstanceSingleCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))

  instance$eval_batch(data.table(x = c(-6, -5, 3, 9)))

  learner = lrn("regr.km",
    covtype = "matern3_2",
    optim.method = "gen",
    nugget.stability = 10^-8,
    control = list(trace = FALSE))

  surrogate = srlrn(learner, archive = instance$archive)

  acq_function = acqf("ei", surrogate = surrogate)

  acq_function$surrogate$update()
  acq_function$update()
  acq_function$eval_dt(data.table(x = c(-1, 0, 1)))
}
```

 mlr_acqfunctions_eips *Acquisition Function Expected Improvement Per Second*

Description

Expected Improvement per Second.

It is assumed that calculations are performed on an `bbotk::OptimInstanceSingleCrit`. Additionally to target values of the codomain that should be minimized or maximized, the `bbotk::Objective` of the `bbotk::OptimInstanceSingleCrit` should return time values. The column names of the target variable and time variable must be passed as `y_cols` in the order (target, time) when constructing the `SurrogateLearnerCollection` that is being used as a surrogate.

Dictionary

This `AcqFunction` can be instantiated via the dictionary `mlr_acqfunctions` or with the associated sugar function `acqf()`:

```
mlr_acqfunctions$get("eips")
acqf("eips")
```

Super classes

```
bbotk::Objective -> mlr3mbo::AcqFunction -> AcqFunctionEIPS
```

Public fields

```
y_best (numeric(1))
  Best objective function value observed so far. In the case of maximization, this already includes the necessary change of sign.
```

Active bindings

```
y_col (character(1)).
time_col (character(1)).
```

Methods

Public methods:

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

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

Usage:

```
AcqFunctionEIPS$new(surrogate = NULL)
```

Arguments:

surrogate (NULL | [SurrogateLearnerCollection](#)).

Method `update()`: Updates acquisition function and sets `y_best`.

Usage:

```
AcqFunctionEIPS$update()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

References

- Snoek, Jasper, Larochelle, Hugo, Adams, P R (2012). “Practical Bayesian Optimization of Machine Learning Algorithms.” In Pereira F, Burges CJC, Bottou L, Weinberger KQ (eds.), *Advances in Neural Information Processing Systems*, volume 25, 2951–2959.

See Also

Other Acquisition Function: [AcqFunction](#), [mlr_acqfunctions_aei](#), [mlr_acqfunctions_cb](#), [mlr_acqfunctions_ei](#), [mlr_acqfunctions_mean](#), [mlr_acqfunctions_pi](#), [mlr_acqfunctions_smsego](#), [mlr_acqfunctions](#)

Examples

```
if (requireNamespace("mlr3learners") &
    requireNamespace("DiceKriging") &
    requireNamespace("rgenoud")) {
  library(bbotk)
  library(paradox)
  library(mlr3learners)
  library(data.table)

  fun = function(xs) {
    list(y = xs$x ^ 2, time = abs(xs$x))
  }
  domain = ps(x = p_dbl(lower = -10, upper = 10))
  codomain = ps(y = p_dbl(tags = "minimize"), time = p_dbl(tags = "time"))
  objective = ObjectiveRFun$new(fun = fun, domain = domain, codomain = codomain)

  instance = OptimInstanceSingleCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))

  instance$eval_batch(data.table(x = c(-6, -5, 3, 9)))

  learner = lrn("regr.km",
    covtype = "matern3_2",
    optim.method = "gen",
    nugget.stability = 10^-8,
```

```

control = list(trace = FALSE))

surrogate = srlrnc(list(learner, learner$clone(deep = TRUE)), archive = instance$archive)
surrogate$y_cols = c("y", "time")

acq_function = acqf("eips", surrogate = surrogate)

acq_function$surrogate$update()
acq_function$update()
acq_function$eval_dt(data.table(x = c(-1, 0, 1)))
}

```

mlr_acqfunctions_mean *Acquisition Function Mean*

Description

Posterior Mean.

Dictionary

This [AcqFunction](#) can be instantiated via the [dictionary mlr_acqfunctions](#) or with the associated sugar function [acqf\(\)](#):

```

mlr_acqfunctions$get("mean")
acqf("mean")

```

Super classes

[bbotk::Objective](#) -> [mlr3mbo::AcqFunction](#) -> [AcqFunctionMean](#)

Methods

Public methods:

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

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

Usage:

```
AcqFunctionMean$new(surrogate = NULL)
```

Arguments:

surrogate (NULL | [SurrogateLearner](#)).

Method [clone\(\)](#): The objects of this class are cloneable with this method.

Usage:

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

Arguments:

deep Whether to make a deep clone.

See Also

Other Acquisition Function: [AcqFunction](#), [mlr_acqfunctions_aei](#), [mlr_acqfunctions_cb](#), [mlr_acqfunctions_eips](#), [mlr_acqfunctions_ei](#), [mlr_acqfunctions_pi](#), [mlr_acqfunctions_smsego](#), [mlr_acqfunctions](#)

Examples

```
if (requireNamespace("mlr3learners") &
    requireNamespace("DiceKriging") &
    requireNamespace("rgenoud")) {
  library(bbotk)
  library(paradox)
  library(mlr3learners)
  library(data.table)

  fun = function(xs) {
    list(y = xs$x ^ 2)
  }
  domain = ps(x = p_dbl(lower = -10, upper = 10))
  codomain = ps(y = p_dbl(tags = "minimize"))
  objective = ObjectiveRfun$new(fun = fun, domain = domain, codomain = codomain)

  instance = OptimInstanceSingleCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))

  instance$eval_batch(data.table(x = c(-6, -5, 3, 9)))

  learner = lrn("regr.km",
    covtype = "matern3_2",
    optim.method = "gen",
    nugget.stability = 10^-8,
    control = list(trace = FALSE))

  surrogate = srlrn(learner, archive = instance$archive)

  acq_function = acqf("mean", surrogate = surrogate)

  acq_function$surrogate$update()
  acq_function$update()
  acq_function$eval_dt(data.table(x = c(-1, 0, 1)))
}
```

mlr_acqfunctions_pi *Acquisition Function Probability of Improvement*

Description

Probability of Improvement.

Dictionary

This [AcqFunction](#) can be instantiated via the [dictionary mlr_acqfunctions](#) or with the associated sugar function `acqf()`:

```
mlr_acqfunctions$get("pi")
acqf("pi")
```

Super classes

[bbotk::Objective](#) -> [mlr3mbo::AcqFunction](#) -> [AcqFunctionPI](#)

Public fields

`y_best` (numeric(1))

Best objective function value observed so far. In the case of maximization, this already includes the necessary change of sign.

Methods**Public methods:**

- [AcqFunctionPI\\$new\(\)](#)
- [AcqFunctionPI\\$update\(\)](#)
- [AcqFunctionPI\\$clone\(\)](#)

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

Usage:

```
AcqFunctionPI$new(surrogate = NULL)
```

Arguments:

`surrogate` (NULL | [SurrogateLearner](#)).

Method `update()`: Updates acquisition function and sets `y_best`.

Usage:

```
AcqFunctionPI$update()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

References

- Kushner, J. H (1964). "A New Method of Locating the Maximum Point of an Arbitrary Multipipeak Curve in the Presence of Noise." *Journal of Basic Engineering*, **86**(1), 97–106.

See Also

Other Acquisition Function: [AcqFunction](#), [mlr_acqfunctions_aei](#), [mlr_acqfunctions_cb](#), [mlr_acqfunctions_eips](#), [mlr_acqfunctions_ei](#), [mlr_acqfunctions_mean](#), [mlr_acqfunctions_smsego](#), [mlr_acqfunctions](#)

Examples

```

if (requireNamespace("mlr3learners") &
    requireNamespace("DiceKriging") &
    requireNamespace("rgenoud")) {
  library(bbotk)
  library(paradox)
  library(mlr3learners)
  library(data.table)

  fun = function(xs) {
    list(y = xs$x ^ 2)
  }
  domain = ps(x = p_dbl(lower = -10, upper = 10))
  codomain = ps(y = p_dbl(tags = "minimize"))
  objective = ObjectiveRFun$new(fun = fun, domain = domain, codomain = codomain)

  instance = OptimInstanceSingleCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))

  instance$eval_batch(data.table(x = c(-6, -5, 3, 9)))

  learner = lrn("regr.km",
    covtype = "matern3_2",
    optim.method = "gen",
    nugget.stability = 10^-8,
    control = list(trace = FALSE))

  surrogate = srlrn(learner, archive = instance$archive)

  acq_function = acqf("pi", surrogate = surrogate)

  acq_function$surrogate$update()
  acq_function$update()
  acq_function$eval_dt(data.table(x = c(-1, 0, 1)))
}

```

mlr_acqfunctions_smsego

Acquisition Function SMS-EGO

Description

S-Metric Selection Evolutionary Multi-Objective Optimization Algorithm Acquisition Function.

Parameters

- "lambda" (numeric(1))
 λ value used for the confidence bound. Defaults to 1. Based on $\text{confidence} = (1 - 2 * \text{dnorm}(\lambda)) ^ m$ you can calculate a lambda for a given confidence level, see Ponweiser et al. (2008).
- "epsilon" (numeric(1))
 ϵ used for the additive epsilon dominance. Can either be a single numeric value > 0 or NULL (default). In the case of being NULL, an epsilon vector is maintained dynamically as described in Horn et al. (2015).

Super classes

`bbotk::Objective` -> `mlr3mbo::AcqFunction` -> `AcqFunctionSmsEgo`

Public fields

`ys_front` (matrix())
 Approximated Pareto front.

`ref_point` (numeric())
 Reference point.

`epsilon` (numeric())
 Epsilon used for the additive epsilon dominance.

`progress` (numeric(1))
 Optimization progress (typically, the number of function evaluations left). Note that this requires the `bbotk::OptimInstance` to be terminated via a `bbotk::TerminatorEvals`.

Methods**Public methods:**

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

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

Usage:

`AcqFunctionSmsEgo$new(surrogate = NULL, lambda = 1, epsilon = NULL)`

Arguments:

`surrogate` (NULL | `SurrogateLearnerCollection`).

`lambda` (numeric(1)).

`epsilon` (NULL | numeric(1)).

Method `update()`: Updates acquisition function and sets `ys_front`, `ref_point`, `epsilon`.

Usage:

`AcqFunctionSmsEgo$update()`

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

Usage:

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

Arguments:

```
deep Whether to make a deep clone.
```

References

- Ponweiser, Wolfgang, Wagner, Tobias, Biermann, Dirk, Vincze, Markus (2008). “Multiobjective Optimization on a Limited Budget of Evaluations Using Model-Assisted S-Metric Selection.” In *Proceedings of the 10th International Conference on Parallel Problem Solving from Nature*, 784–794.
- Horn, Daniel, Wagner, Tobias, Biermann, Dirk, Weihs, Claus, Bischl, Bernd (2015). “Model-Based Multi-objective Optimization: Taxonomy, Multi-Point Proposal, Toolbox and Benchmark.” In *International Conference on Evolutionary Multi-Criterion Optimization*, 64–78.

See Also

Other Acquisition Function: [AcqFunction](#), [mlr_acqfunctions_aei](#), [mlr_acqfunctions_cb](#), [mlr_acqfunctions_eips](#), [mlr_acqfunctions_ei](#), [mlr_acqfunctions_mean](#), [mlr_acqfunctions_pi](#), [mlr_acqfunctions](#)

Examples

```
if (requireNamespace("mlr3learners") &
    requireNamespace("DiceKriging") &
    requireNamespace("rgenoud")) {
  library(bbotk)
  library(paradox)
  library(mlr3learners)
  library(data.table)

  fun = function(xs) {
    list(y1 = xs$x^2, y2 = (xs$x - 2) ^ 2)
  }
  domain = ps(x = p_dbl(lower = -10, upper = 10))
  codomain = ps(y1 = p_dbl(tags = "minimize"), y2 = p_dbl(tags = "minimize"))
  objective = ObjectiveRfun$new(fun = fun, domain = domain, codomain = codomain)

  instance = OptimInstanceMultiCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))

  instance$eval_batch(data.table(x = c(-6, -5, 3, 9)))

  learner = lrn("regr.km",
    covtype = "matern3_2",
    optim.method = "gen",
    nugget.stability = 10^-8,
    control = list(trace = FALSE))

  surrogate = srlrnc(list(learner, learner$clone(deep = TRUE)), archive = instance$archive)
```

```
acq_function = acqf("smsego", surrogate = surrogate)

acq_function$surrogate$update()
acq_function$progress = 5 - 4 # n_evals = 5 and 4 points already evaluated
acq_function$update()
acq_function$eval_dt(data.table(x = c(-1, 0, 1)))
}
```

mlr_loop_functions *Dictionary of Loop Functions*

Description

A simple [mlr3misc::Dictionary](#) storing objects of class `loop_function`. Each loop function has an associated help page, see `mlr_loop_functions_[id]`.

Retrieves object with key `key` from the dictionary. Additional arguments must be named and are passed to the constructor of the stored object.

Arguments

<code>key</code>	(character(1)).
<code>...</code>	(any) Passed down to constructor.

Format

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

Value

Object with corresponding key.

Methods

See [mlr3misc::Dictionary](#).

See Also

Other Dictionary: [mlr_acqfunctions](#)

Other Loop Function: [loop_function](#), [mlr_loop_functions_ego](#), [mlr_loop_functions_mpl](#), [mlr_loop_functions_parego](#), [mlr_loop_functions_smsego](#)

Examples

```
as.data.table(mlr_loop_functions)
```

mlr_loop_functions_ego

Sequential Single-Objective Bayesian Optimization

Description

Loop function for sequential single-objective Bayesian Optimization. Normally used inside an [OptimizerMbo](#).

In each iteration after the initial design, the surrogate and acquisition function are updated and the next candidate is chosen based on optimizing the acquisition function.

Usage

```

bayesopt_ego(
  instance,
  init_design_size = NULL,
  surrogate,
  acq_function,
  acq_optimizer,
  random_interleave_iter = 0L
)

```

Arguments

instance	(bbotk::OptimInstanceSingleCrit) The bbotk::OptimInstanceSingleCrit to be optimized.
init_design_size	(NULL integer(1)) Size of the initial design. If NULL and the bbotk::Archive contains no evaluations, $4 * d$ is used with d being the dimensionality of the search space. Points are drawn uniformly at random.
surrogate	(Surrogate) Surrogate to be used as a surrogate. Typically a SurrogateLearner .
acq_function	(AcqFunction) AcqFunction to be used as acquisition function.
acq_optimizer	(AcqOptimizer) AcqOptimizer to be used as acquisition function optimizer.
random_interleave_iter	(integer(1)) Every <code>random_interleave_iter</code> iteration (starting after the initial design), a point is sampled uniformly at random and evaluated (instead of a model based proposal). For example, if <code>random_interleave_iter = 2</code> , random interleaving is performed in the second, fourth, sixth, ... iteration. Default is 0, i.e., no random interleaving is performed at all.

Value

invisible(instance)

The original instance is modified in-place and returned invisible.

Note

- The `acq_function$surrogate`, even if already populated, will always be overwritten by the surrogate.
- The `acq_optimizer$acq_function`, even if already populated, will always be overwritten by `acq_function`.
- The `surrogate$archive`, even if already populated, will always be overwritten by the [bbotk::Archive](#) of the [bbotk::OptimInstanceSingleCrit](#).

References

- Jones, R. D, Schonlau, Matthias, Welch, J. W (1998). “Efficient Global Optimization of Expensive Black-Box Functions.” *Journal of Global optimization*, **13**(4), 455–492.
- Snoek, Jasper, Larochelle, Hugo, Adams, P R (2012). “Practical Bayesian Optimization of Machine Learning Algorithms.” In Pereira F, Burges CJC, Bottou L, Weinberger KQ (eds.), *Advances in Neural Information Processing Systems*, volume 25, 2951–2959.

See Also

Other Loop Function: [loop_function](#), [mlr_loop_functions_mpc1](#), [mlr_loop_functions_parego](#), [mlr_loop_functions_smsego](#), [mlr_loop_functions](#)

Examples

```
if (requireNamespace("mlr3learners") &
    requireNamespace("DiceKriging") &
    requireNamespace("rgenoud")) {

  library(bbotk)
  library(paradox)
  library(mlr3learners)

  fun = function(xs) {
    list(y = xs$x ^ 2)
  }
  domain = ps(x = p_dbl(lower = -10, upper = 10))
  codomain = ps(y = p_dbl(tags = "minimize"))
  objective = ObjectiveRfun$new(fun = fun, domain = domain, codomain = codomain)

  instance = OptimInstanceSingleCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))

  surrogate = default_surrogate(instance)
```

```

acq_function = acqf("ei")

acq_optimizer = acqo(
  optimizer = opt("random_search", batch_size = 100),
  terminator = trm("evals", n_evals = 100))

optimizer = opt("mbo",
  loop_function = bayesopt_ego,
  surrogate = surrogate,
  acq_function = acq_function,
  acq_optimizer = acq_optimizer)

optimizer$optimize(instance)

# expected improvement per second example
fun = function(xs) {
  list(y = xs$x ^ 2, time = abs(xs$x))
}
domain = ps(x = p_dbl(lower = -10, upper = 10))
codomain = ps(y = p_dbl(tags = "minimize"), time = p_dbl(tags = "time"))
objective = ObjectiveRfun$new(fun = fun, domain = domain, codomain = codomain)

instance = OptimInstanceSingleCrit$new(
  objective = objective,
  terminator = trm("evals", n_evals = 5))

surrogate = default_surrogate(instance, n_learner = 2)
surrogate$y_cols = c("y", "time")

optimizer = opt("mbo",
  loop_function = bayesopt_ego,
  surrogate = surrogate,
  acq_function = acqf("eips"),
  acq_optimizer = acq_optimizer)

optimizer$optimize(instance)
}

```

mlr_loop_functions_mpc1

Single-Objective Bayesian Optimization via Multipoint Constant Liars

Description

Loop function for single-objective Bayesian Optimization via multipoint constant liar. Normally used inside an [OptimizerMbo](#).

In each iteration after the initial design, the surrogate and acquisition function are updated. The acquisition function is then optimized, to find a candidate but instead of evaluating this candidate,

the objective function value is obtained by applying the `liar` function to all previously obtained objective function values. This is repeated $q - 1$ times to obtain a total of q candidates that are then evaluated in a single batch.

Usage

```
bayesopt_mpcl(
  instance,
  init_design_size = NULL,
  surrogate,
  acq_function,
  acq_optimizer,
  q = 2L,
  liar = mean,
  random_interleave_iter = 0L
)
```

Arguments

<code>instance</code>	(bbotk::OptimInstanceSingleCrit) The bbotk::OptimInstanceSingleCrit to be optimized.
<code>init_design_size</code>	(<code>NULL</code> <code>integer(1)</code>) Size of the initial design. If <code>NULL</code> and the bbotk::Archive contains no evaluations, $4 * d$ is used with d being the dimensionality of the search space. Points are drawn uniformly at random.
<code>surrogate</code>	(Surrogate) Surrogate to be used as a surrogate. Typically a SurrogateLearner .
<code>acq_function</code>	(AcqFunction) AcqFunction to be used as acquisition function.
<code>acq_optimizer</code>	(AcqOptimizer) AcqOptimizer to be used as acquisition function optimizer.
<code>q</code>	(<code>integer(1)</code>) Batch size > 1. Default is 2.
<code>liar</code>	(function) Any function accepting a numeric vector as input and returning a single numeric output. Default is <code>mean</code> . Other sensible functions include <code>min</code> (or <code>max</code> , depending on the optimization direction).
<code>random_interleave_iter</code>	(<code>integer(1)</code>) Every <code>random_interleave_iter</code> iteration (starting after the initial design), a point is sampled uniformly at random and evaluated (instead of a model based proposal). For example, if <code>random_interleave_iter = 2</code> , random interleaving is performed in the second, fourth, sixth, ... iteration. Default is 0, i.e., no random interleaving is performed at all.

Value

invisible(instance)

The original instance is modified in-place and returned invisible.

Note

- The `acq_function$surrogate`, even if already populated, will always be overwritten by the surrogate.
- The `acq_optimizer$acq_function`, even if already populated, will always be overwritten by `acq_function`.
- The `surrogate$archive`, even if already populated, will always be overwritten by the [bbotk::Archive](#) of the [bbotk::OptimInstanceSingleCrit](#).
- To make use of parallel evaluations in the case of $q > 1$, the objective function of the [bbotk::OptimInstanceSingleCrit](#) must be implemented accordingly.

References

- Ginsbourger, David, Le Riche, Rodolphe, Carraro, Laurent (2008). “A Multi-Points Criterion for Deterministic Parallel Global Optimization Based on Gaussian Processes.”
- Wang, Jialei, Clark, C. S, Liu, Eric, Frazier, I. P (2020). “Parallel Bayesian Global Optimization of Expensive Functions.” *Operations Research*, **68**(6), 1850–1865.

See Also

Other Loop Function: [loop_function](#), [mlr_loop_functions_ego](#), [mlr_loop_functions_parego](#), [mlr_loop_functions_smsego](#), [mlr_loop_functions](#)

Examples

```
if (requireNamespace("mlr3learners") &
    requireNamespace("DiceKriging") &
    requireNamespace("rgenoud")) {

  library(bbotk)
  library(paradox)
  library(mlr3learners)

  fun = function(xs) {
    list(y = xs$x ^ 2)
  }
  domain = ps(x = p_dbl(lower = -10, upper = 10))
  codomain = ps(y = p_dbl(tags = "minimize"))
  objective = ObjectiveRFun$new(fun = fun, domain = domain, codomain = codomain)

  instance = OptimInstanceSingleCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 7))
}
```

```

surrogate = default_surrogate(instance)

acq_function = acqf("ei")

acq_optimizer = acqo(
  optimizer = opt("random_search", batch_size = 100),
  terminator = trm("evals", n_evals = 100))

optimizer = opt("mbo",
  loop_function = bayesopt_mpcl,
  surrogate = surrogate,
  acq_function = acq_function,
  acq_optimizer = acq_optimizer,
  args = list(q = 3))

optimizer$optimize(instance)
}

```

mlr_loop_functions_parego

Multi-Objective Bayesian Optimization via ParEGO

Description

Loop function for multi-objective Bayesian Optimization via ParEGO. Normally used inside an [OptimizerMbo](#).

In each iteration after the initial design, the observed objective function values are normalized and q candidates are obtained by scalarizing these values via the augmented Tchebycheff function, updating the surrogate with respect to these scalarized values and optimizing the acquisition function.

Usage

```

bayesopt_parego(
  instance,
  init_design_size = NULL,
  surrogate,
  acq_function,
  acq_optimizer,
  q = 1L,
  s = 100L,
  rho = 0.05,
  random_interleave_iter = 0L
)

```

Arguments

instance	(bbotk::OptimInstanceMultiCrit) The bbotk::OptimInstanceMultiCrit to be optimized.
init_design_size	(NULL integer(1)) Size of the initial design. If NULL and the bbotk::Archive contains no evaluations, $4 * d$ is used with d being the dimensionality of the search space. Points are drawn uniformly at random.
surrogate	(SurrogateLearner) SurrogateLearner to be used as a surrogate.
acq_function	(AcqFunction) AcqFunction to be used as acquisition function.
acq_optimizer	(AcqOptimizer) AcqOptimizer to be used as acquisition function optimizer.
q	(integer(1)) Batch size, i.e., the number of candidates to be obtained for a single batch. Default is 1.
s	(integer(1)) s in Equation 1 in Knowles (2006). Determines the total number of possible random weight vectors. Default is 100.
rho	(numeric(1)) ρ in Equation 2 in Knowles (2006) scaling the linear part of the augmented Tchebycheff function. Default is 0.05
random_interleave_iter	(integer(1)) Every <code>random_interleave_iter</code> iteration (starting after the initial design), a point is sampled uniformly at random and evaluated (instead of a model based proposal). For example, if <code>random_interleave_iter = 2</code> , random interleaving is performed in the second, fourth, sixth, ... iteration. Default is 0, i.e., no random interleaving is performed at all.

Value

`invisible(instance)`
The original instance is modified in-place and returned invisible.

Note

- The `acq_function$surrogate`, even if already populated, will always be overwritten by the surrogate.
- The `acq_optimizer$acq_function`, even if already populated, will always be overwritten by `acq_function`.
- The `surrogate$archive`, even if already populated, will always be overwritten by the [bbotk::Archive](#) of the [bbotk::OptimInstanceMultiCrit](#).
- The scalarizations of the objective function values are stored as the `y_scal` column in the [bbotk::Archive](#) of the [bbotk::OptimInstanceMultiCrit](#).

- To make use of parallel evaluations in the case of $q > 1$, the objective function of the `bbotk::OptimInstanceMultiCrit` must be implemented accordingly.

References

- Knowles, Joshua (2006). “ParEGO: A Hybrid Algorithm With On-Line Landscape Approximation for Expensive Multiobjective Optimization Problems.” *IEEE Transactions on Evolutionary Computation*, **10**(1), 50–66.

See Also

Other Loop Function: [loop_function](#), [mlr_loop_functions_ego](#), [mlr_loop_functions_mpcl](#), [mlr_loop_functions_smsego](#), [mlr_loop_functions](#)

Examples

```
if (requireNamespace("mlr3learners") &
    requireNamespace("DiceKriging") &
    requireNamespace("rgenoud")) {

  library(bbotk)
  library(paradox)
  library(mlr3learners)

  fun = function(xs) {
    list(y1 = xs$x^2, y2 = (xs$x - 2) ^ 2)
  }
  domain = ps(x = p_dbl(lower = -10, upper = 10))
  codomain = ps(y1 = p_dbl(tags = "minimize"), y2 = p_dbl(tags = "minimize"))
  objective = ObjectiveRfun$new(fun = fun, domain = domain, codomain = codomain)

  instance = OptimInstanceMultiCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))

  surrogate = default_surrogate(instance, n_learner = 1)

  acq_function = acqf("ei")

  acq_optimizer = acqo(
    optimizer = opt("random_search", batch_size = 100),
    terminator = trm("evals", n_evals = 100))

  optimizer = opt("mbo",
    loop_function = bayesopt_parego,
    surrogate = surrogate,
    acq_function = acq_function,
    acq_optimizer = acq_optimizer)

  optimizer$optimize(instance)
}
```

mlr_loop_functions_smsego

Sequential Multi-Objective Bayesian Optimization via SMS-EGO

Description

Loop function for sequential multi-objective Bayesian Optimization via SMS-EGO. Normally used inside an [OptimizerMbo](#).

In each iteration after the initial design, the surrogate and acquisition function ([mlr_acqfunctions_smsego](#)) are updated and the next candidate is chosen based on optimizing the acquisition function.

Usage

```
bayesopt_smsego(
  instance,
  init_design_size = NULL,
  surrogate,
  acq_function,
  acq_optimizer,
  random_interleave_iter = 0L
)
```

Arguments

instance	(bbotk::OptimInstanceMultiCrit) The bbotk::OptimInstanceMultiCrit to be optimized.
init_design_size	(NULL integer(1)) Size of the initial design. If NULL and the bbotk::Archive contains no evaluations, $4 * d$ is used with d being the dimensionality of the search space. Points are drawn uniformly at random.
surrogate	(SurrogateLearnerCollection) SurrogateLearnerCollection to be used as a surrogate.
acq_function	(mlr_acqfunctions_smsego) mlr_acqfunctions_smsego to be used as acquisition function.
acq_optimizer	(AcqOptimizer) AcqOptimizer to be used as acquisition function optimizer.
random_interleave_iter	(integer(1)) Every <code>random_interleave_iter</code> iteration (starting after the initial design), a point is sampled uniformly at random and evaluated (instead of a model based proposal). For example, if <code>random_interleave_iter = 2</code> , random interleaving is performed in the second, fourth, sixth, ... iteration. Default is 0, i.e., no random interleaving is performed at all.

Value

invisible(instance)

The original instance is modified in-place and returned invisible.

Note

- The `acq_function$surrogate`, even if already populated, will always be overwritten by the `surrogate`.
- The `acq_optimizer$acq_function`, even if already populated, will always be overwritten by `acq_function`.
- The `surrogate$archive`, even if already populated, will always be overwritten by the `bbotk::Archive` of the `bbotk::OptimInstanceMultiCrit`.
- Due to the iterative computation of the epsilon within the `mlr_acqfunctions_smsego`, requires the `bbotk::Terminator` of the `bbotk::OptimInstanceMultiCrit` to be a `bbotk::TerminatorEvals`.

References

- Beume N, Naujoks B, Emmerich M (2007). “SMS-EMOA: Multiobjective selection based on dominated hypervolume.” *European Journal of Operational Research*, **181**(3), 1653–1669.
- Ponweiser, Wolfgang, Wagner, Tobias, Biermann, Dirk, Vincze, Markus (2008). “Multiobjective Optimization on a Limited Budget of Evaluations Using Model-Assisted S-Metric Selection.” In *Proceedings of the 10th International Conference on Parallel Problem Solving from Nature*, 784–794.

See Also

Other Loop Function: [loop_function](#), [mlr_loop_functions_ego](#), [mlr_loop_functions_mpcl](#), [mlr_loop_functions_parego](#), [mlr_loop_functions](#)

Examples

```
if (requireNamespace("mlr3learners") &
    requireNamespace("DiceKriging") &
    requireNamespace("rgenoud")) {

  library(bbotk)
  library(paradox)
  library(mlr3learners)

  fun = function(xs) {
    list(y1 = xs$x^2, y2 = (xs$x - 2) ^ 2)
  }
  domain = ps(x = p_dbl(lower = -10, upper = 10))
  codomain = ps(y1 = p_dbl(tags = "minimize"), y2 = p_dbl(tags = "minimize"))
  objective = ObjectiveRfun$new(fun = fun, domain = domain, codomain = codomain)

  instance = OptimInstanceMultiCrit$new(
    objective = objective,
```

```

    terminator = trm("evals", n_evals = 5))

surrogate = default_surrogate(instance)

acq_function = acqf("smsego")

acq_optimizer = acqo(
  optimizer = opt("random_search", batch_size = 100),
  terminator = trm("evals", n_evals = 100))

optimizer = opt("mbo",
  loop_function = bayesopt_smsego,
  surrogate = surrogate,
  acq_function = acq_function,
  acq_optimizer = acq_optimizer)

optimizer$optimize(instance)
}

```

mlr_optimizers_mbo *Model Based Optimization*

Description

OptimizerMbo class that implements Model Based Optimization (MBO). The implementation follows a modular layout relying on a [loop_function](#) determining the MBO flavor to be used, e.g., [bayesopt_ego](#) for sequential single-objective Bayesian Optimization, a [Surrogate](#), an [AcqFunction](#), e.g., [mlr_acqfunctions_ei](#) for Expected Improvement and an [AcqOptimizer](#).

MBO algorithms are iterative optimization algorithms that make use of a continuously updated surrogate model built for the objective function. By optimizing a comparably cheap to evaluate acquisition function defined on the surrogate prediction, the next candidate is chosen for evaluation. Detailed descriptions of different MBO flavors are provided in the documentation of the respective [loop_function](#).

Termination is handled via a [bbotk::Terminator](#) part of the [bbotk::OptimInstance](#) to be optimized.

Archive

The [bbotk::Archive](#) holds the following additional columns that are specific to MBO algorithms:

- `[acq_function$id]` (`numeric(1)`)
The value of the acquisition function.
- `.already_evaluated` (`logical(1)`)
Whether this point was already evaluated. Depends on the `skip_already_evaluated` parameter of the [AcqOptimizer](#).

Super class

[bbotk::Optimizer](#) -> OptimizerMbo

Active bindings

- `loop_function` ([loop_function](#) | NULL)
Loop function determining the MBO flavor.
- `surrogate` ([Surrogate](#) | NULL)
The surrogate.
- `acq_function` ([AcqFunction](#) | NULL)
The acquisition function.
- `acq_optimizer` ([AcqOptimizer](#) | NULL)
The acquisition function optimizer.
- `args` (named `list()`)
Further arguments passed to the `loop_function`. For example, `random_interleave_iter`.
- `result_function` (`function` | NULL)
Optional function called after the optimization terminates. Determines how the final result of the optimization is calculated. Requires arguments `inst` (the [bbotk::OptimInstance](#)) and `self` (the [OptimizerMbo](#)). See for example [result_by_surrogate_design](#) which is used by default if the [bbotk::OptimInstance](#) has the property "noisy" (which is the case for a [mlr3tuning::TuningInstanceSingleCrit](#) or [mlr3tuning::TuningInstanceMultiCrit](#)).
- `param_classes` (`character()`)
Supported parameter classes that the optimizer can optimize. Determined based on the surrogate and the `acq_optimizer`. Subclasses of [paradox::Param](#).
- `properties` (`character()`)
Set of properties of the optimizer. Must be a subset of [bbotk_reflections\\$optimizer_properties](#). MBO in principle is very flexible and by default we assume that the optimizer has all properties. When fully initialized, properties are determined based on the `loop_function` and surrogate.
- `packages` (`character()`)
Set of required packages. A warning is signaled prior to optimization if at least one of the packages is not installed, but loaded (not attached) later on-demand via [requireNamespace\(\)](#). Required packages are determined based on the surrogate and the `acq_optimizer`.

Methods**Public methods:**

- [OptimizerMbo\\$new\(\)](#)
- [OptimizerMbo\\$print\(\)](#)
- [OptimizerMbo\\$reset\(\)](#)
- [OptimizerMbo\\$clone\(\)](#)

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

If `surrogate` is NULL and the `acq_function$surrogate` field is populated, this [Surrogate](#) is used. Otherwise, `default_surrogate(instance)` is used. If `acq_function` is NULL and the `acq_optimizer$acq_function` field is populated, this [AcqFunction](#) is used (and therefore its `$surrogate` if populated; see above). Otherwise `default_acqfun(instance)` is used. If `acq_optimizer` is NULL, `default_acqopt(instance)` is used.

Even if already initialized, the `$surrogate$archive` field will always be overwritten by the `bbotk::Archive` of the current `bbotk::OptimInstance` to be optimized.

For more information on default values for `loop_function`, `surrogate`, `acq_function` and `acq_optimizer`, see `?mbo_defaults`.

Usage:

```
OptimizerMbo$new(
  loop_function = NULL,
  surrogate = NULL,
  acq_function = NULL,
  acq_optimizer = NULL,
  args = NULL,
  result_function = NULL
)
```

Arguments:

`loop_function` (`loop_function` | `NULL`)

Loop function determining the MBO flavor.

`surrogate` (`Surrogate` | `NULL`)

The surrogate.

`acq_function` (`AcqFunction` | `NULL`)

The acquisition function.

`acq_optimizer` (`AcqOptimizer` | `NULL`)

The acquisition function optimizer.

`args` (named `list()`)

Further arguments passed to the `loop_function`. For example, `random_interleave_iter`.

`result_function` (`function` | `NULL`)

Optional function called after the optimization terminates. Determines how the final result of the optimization is calculated. Requires arguments `inst` (the `bbotk::OptimInstance`) and `self` (the `OptimizerMbo`). See for example `result_by_surrogate_design` which is used by default if the `bbotk::OptimInstance` has the property "noisy" (which is the case for a `mlr3tuning::TuningInstanceSingleCrit` or `mlr3tuning::TuningInstanceMultiCrit`).

Method `print()`: Print method.

Usage:

```
OptimizerMbo$print()
```

Returns: (`character()`).

Method `reset()`: Reset the optimizer. Sets the following fields to `NULL`: `loop_function`, `surrogate`, `acq_function`, `acq_optimizer`, `args`, `result_function`

Usage:

```
OptimizerMbo$reset()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Examples

```

if (requireNamespace("mlr3learners") &
    requireNamespace("DiceKriging") &
    requireNamespace("rgenoud")) {

  library(bbotk)
  library(paradox)
  library(mlr3learners)

  # single-objective EGO
  fun = function(xs) {
    list(y = xs$x ^ 2)
  }
  domain = ps(x = p_dbl(lower = -10, upper = 10))
  codomain = ps(y = p_dbl(tags = "minimize"))
  objective = ObjectiveRFun$new(fun = fun, domain = domain, codomain = codomain)

  instance = OptimInstanceSingleCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))

  learner = lrn("regr.km",
    covtype = "matern3_2",
    optim.method = "gen",
    nugget.stability = 10^-8,
    control = list(trace = FALSE))

  surrogate = srlrn(learner)

  acq_function = acqf("ei")

  acq_optimizer = acqo(
    optimizer = opt("random_search", batch_size = 100),
    terminator = trm("evals", n_evals = 100))

  optimizer = opt("mbo",
    loop_function = bayesopt_ego,
    surrogate = surrogate,
    acq_function = acq_function,
    acq_optimizer = acq_optimizer)

  optimizer$optimize(instance)

  # multi-objective ParEGO
  fun = function(xs) {
    list(y1 = xs$x^2, y2 = (xs$x - 2) ^ 2)
  }
  domain = ps(x = p_dbl(lower = -10, upper = 10))
  codomain = ps(y1 = p_dbl(tags = "minimize"), y2 = p_dbl(tags = "minimize"))
  objective = ObjectiveRFun$new(fun = fun, domain = domain, codomain = codomain)

```

```

instance = OptimInstanceMultiCrit$new(
  objective = objective,
  terminator = trm("evals", n_evals = 5))

optimizer = opt("mbo",
  loop_function = bayesopt_parego,
  surrogate = surrogate,
  acq_function = acq_function,
  acq_optimizer = acq_optimizer)

optimizer$optimize(instance)
}

```

mlr_tuners_mbo

Tuner using Model Based Optimization

Description

TunerMbo class that implements Model Based Optimization (MBO). This is a minimal interface internally passing on to [OptimizerMbo](#). For additional information and documentation see [OptimizerMbo](#).

Super classes

```
mlr3tuning::Tuner -> mlr3tuning::TunerFromOptimizer -> TunerMbo
```

Active bindings

```
loop_function (loop_function | NULL)
  Loop function determining the MBO flavor.

surrogate (Surrogate | NULL)
  The surrogate.

acq_function (AcqFunction | NULL)
  The acquisition function.

acq_optimizer (AcqOptimizer | NULL)
  The acquisition function optimizer.

args (named list())
  Further arguments passed to the loop_function. For example, random_interleave_iter.

result_function (function | NULL)
  Optional function called after the optimization terminates. Determines how the final result of the optimization is calculated. Requires arguments inst (the bbotk::OptimInstance) and self (the OptimizerMbo). See for example result\_by\_surrogate\_design which is used by default if the bbotk::OptimInstance has the property "noisy" (which is the case for a mlr3tuning::TuningInstanceSingleCrit or mlr3tuning::TuningInstanceMultiCrit).
```

param_classes (character())

Supported parameter classes that the optimizer can optimize. Determined based on the surrogate and the acq_optimizer. Subclasses of [paradox::Param](#).

properties (character())

Set of properties of the optimizer. Must be a subset of [bbotk_reflections\\$optimizer_properties](#). MBO in principle is very flexible and by default we assume that the optimizer has all properties. When fully initialized, properties are determined based on the loop_function and surrogate.

packages (character())

Set of required packages. A warning is signaled prior to optimization if at least one of the packages is not installed, but loaded (not attached) later on-demand via [requireNamespace\(\)](#). Required packages are determined based on the surrogate and the acq_optimizer.

Methods

Public methods:

- [TunerMbo\\$new\(\)](#)
- [TunerMbo\\$print\(\)](#)
- [TunerMbo\\$reset\(\)](#)
- [TunerMbo\\$clone\(\)](#)

Method new(): Creates a new instance of this R6 class. For more information on default values for loop_function, surrogate, acq_function and acq_optimizer, see [?mbo_defaults](#).

Note that all the parameters below are simply passed to the [OptimizerMbo](#) and the respective fields are simply (settable) active bindings to the fields of the [OptimizerMbo](#).

Usage:

```
TunerMbo$new(
  loop_function = NULL,
  surrogate = NULL,
  acq_function = NULL,
  acq_optimizer = NULL,
  args = NULL,
  result_function = NULL
)
```

Arguments:

loop_function ([loop_function](#) | NULL)

Loop function determining the MBO flavor.

surrogate ([Surrogate](#) | NULL)

The surrogate.

acq_function ([AcqFunction](#) | NULL)

The acquisition function.

acq_optimizer ([AcqOptimizer](#) | NULL)

The acquisition function optimizer.

args (named list())

Further arguments passed to the loop_function. For example, [random_interleave_iter](#).

`result_function` (function|NULL)

Optional function called after the optimization terminates. Determines how the final result of the optimization is calculated. Requires arguments `inst` (the `bbotk::OptimInstance`) and `self` (the `OptimizerMbo`). See for example `result_by_surrogate_design` which is used by default if the `bbotk::OptimInstance` has the property "noisy" (which is the case for a `mlr3tuning::TuningInstanceSingleCrit` or `mlr3tuning::TuningInstanceMultiCrit`).

Method `print()`: Print method.

Usage:

```
TunerMbo$print()
```

Returns: (character()).

Method `reset()`: Reset the tuner. Sets the following fields to NULL: `loop_function`, `surrogate`, `acq_function`, `acq_optimizer`, `args`, `result_function`

Usage:

```
TunerMbo$reset()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Examples

```
if (requireNamespace("mlr3learners") &
    requireNamespace("DiceKriging") &
    requireNamespace("rgenoud")) {

  library(mlr3)
  library(mlr3tuning)

  # single-objective
  task = tsk("wine")
  learner = lrn("classif.rpart", cp = to_tune(lower = 1e-4, upper = 1, logscale = TRUE))
  resampling = rsmpl("cv", folds = 3)
  measure = msr("classif.acc")

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

  tnr("mbo")$optimize(instance)

  # multi-objective
```

```

task = tsk("wine")
learner = lrn("classif.rpart", cp = to_tune(lower = 1e-4, upper = 1, logscale = TRUE))
resampling = rsmp("cv", folds = 3)
measures = msrs(c("classif.acc", "selected_features"))

instance = TuningInstanceMultiCrit$new(
  task = task,
  learner = learner,
  resampling = resampling,
  measures = measures,
  terminator = trm("evals", n_evals = 5),
  store_models = TRUE) # required due to selected features

tnr("mbo")$optimize(instance)
}

```

result_by_default	<i>Choose Final Point(s) based on the Archive</i>
-------------------	---

Description

Choose final point(s) based on all evaluations in the archive.

Usage

```
result_by_default(instance, optimizer_mbo)
```

Arguments

instance	(bbotk::OptimInstanceSingleCrit bbotk::OptimInstanceMultiCrit) The bbotk::OptimInstance the result should be assigned to.
optimizer_mbo	(OptimizerMbo) The OptimizerMbo that generates the final result.

result_by_surrogate_design	<i>Choose Final Point(s) by Surrogate Mean</i>
----------------------------	--

Description

Choose final point(s) by best surrogate mean prediction on all evaluated points.

Usage

```
result_by_surrogate_design(instance, optimizer_mbo)
```

Arguments

instance	(bbotk::OptimInstanceSingleCrit bbotk::OptimInstanceMultiCrit) The bbotk::OptimInstance the result should be assigned to.
optimizer_mbo	(OptimizerMbo) The OptimizerMbo that generates the final result.

srlrn

Syntactic Sugar Surrogate Learner Construction

Description

This function allows to construct a [SurrogateLearner](#) in the spirit of `mlr_sugar` from **mlr3**.

Usage

```
srlrn(learner, archive = NULL, x_cols = NULL, y_col = NULL, ...)
```

Arguments

learner	(mlr3::LearnerRegr) mlr3::LearnerRegr that is to be used.
archive	(NULL bbotk::Archive) bbotk::Archive of the bbotk::OptimInstance used. Can also be NULL.
x_cols	(NULL <code>character()</code>) Names of columns in the bbotk::Archive that should be used as features. Can also be NULL.
y_col	(NULL <code>character(1)</code>) Name of the column in the bbotk::Archive that should be used as a target. Can also be NULL.
...	(<code>named list()</code>) Named arguments passed to the constructor, to be set as parameters in the paradox::ParamSet .

Value

[SurrogateLearner](#)

Examples

```
srlrn(lrn("regr.featureless"), catch_errors = FALSE)
```


srlrnc

*Syntactic Sugar Surrogate Learner Collection Construction***Description**

This function allows to construct a [SurrogateLearnerCollection](#) in the spirit of `mlr_sugar` from **mlr3**.

Usage

```
srlrnc(learners, archive = NULL, x_cols = NULL, y_cols = NULL, ...)
```

Arguments

<code>learners</code>	(List of mlr3::LearnerRegr) mlr3::LearnerRegr that are to be used.
<code>archive</code>	(NULL bbotk::Archive) bbotk::Archive of the bbotk::OptimInstance used. Can also be NULL.
<code>x_cols</code>	(NULL <code>character()</code>) Names of columns in the bbotk::Archive that should be used as features. Can also be NULL.
<code>y_cols</code>	(NULL <code>character()</code>) Names of the columns in the bbotk::Archive that should be used as targets. Can also be NULL.
<code>...</code>	(named <code>list()</code>) Named arguments passed to the constructor, to be set as parameters in the paradox::ParamSet .

Value

[SurrogateLearnerCollection](#)

Examples

```
srlrnc(list(lrn("regr.featureless"), lrn("regr.featureless")), catch_errors = FALSE)
```

 Surrogate

Surrogate Model

Description

Abstract surrogate model class.

A surrogate model is used to model the unknown objective function(s) based on all points evaluated so far.

Public fields

model (model)
Arbitrary model object depending on the subclass.

Active bindings

print_id (character)
Id used when printing.

archive ([bbotk::Archive](#) | NULL)
[bbotk::Archive](#) of the [bbotk::OptimInstance](#).

n_learner (integer(1))
Returns the number of surrogate models.

x_cols (character() | NULL)
Column Id's of variables that should be used as features. By default, automatically inferred based on the archive.

y_cols (character() | NULL)
Column Id's of variables that should be used as targets. By default, automatically inferred based on the archive.

insample_perf (numeric())
Surrogate model's current insample performance.

param_set ([paradox::ParamSet](#))
Set of hyperparameters.

assert_insampl_perf (numeric())
Asserts whether the current insample performance meets the performance threshold.

packages (character())
Set of required packages. A warning is signaled if at least one of the packages is not installed, but loaded (not attached) later on-demand via [requireNamespace\(\)](#).

feature_types (character())
Stores the feature types the surrogate can handle, e.g. "logical", "numeric", or "factor". A complete list of candidate feature types, grouped by task type, is stored in [mlr_reflections\\$task_feature_types](#).

properties (character())
Stores a set of properties/capabilities the surrogate has. A complete list of candidate properties, grouped by task type, is stored in [mlr_reflections\\$learner_properties](#).

predict_type (character(1))
Retrieves the currently active predict type, e.g. "response".

Methods**Public methods:**

- [Surrogate\\$new\(\)](#)
- [Surrogate\\$update\(\)](#)
- [Surrogate\\$predict\(\)](#)
- [Surrogate\\$format\(\)](#)
- [Surrogate\\$print\(\)](#)
- [Surrogate\\$clone\(\)](#)

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

Usage:

```
Surrogate$new(model, archive, x_cols, y_cols, param_set)
```

Arguments:

`model` (model)

Arbitrary model object depending on the subclass.

`archive` ([bbotk::Archive](#) | NULL)

[bbotk::Archive](#) of the [bbotk::OptimInstance](#).

`x_cols` (character() | NULL)

Column Id's of variables that should be used as features. By default, automatically inferred based on the archive.

`y_cols` (character() | NULL)

Column Id's of variables that should be used as targets. By default, automatically inferred based on the archive.

`param_set` ([paradox::ParamSet](#))

Parameter space description depending on the subclass.

Method `update()`: Train model with new data. Subclasses must implement `$private.update()`.

Usage:

```
Surrogate$update()
```

Returns: NULL.

Method `predict()`: Predict mean response and standard error. Must be implemented by subclasses.

Usage:

```
Surrogate$predict(xdt)
```

Arguments:

`xdt` ([data.table::data.table\(\)](#))

New data. One row per observation.

Returns: Arbitrary prediction object.

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

Usage:

```
Surrogate$format()
```

Method `print()`: Print method.

Usage:

`Surrogate$print()`

Returns: (character()).

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

Usage:

`Surrogate$clone(deep = FALSE)`

Arguments:

`deep` Whether to make a deep clone.

SurrogateLearner *Surrogate Model Containing a Single Learner*

Description

Surrogate model containing a single [mlr3::LearnerRegr](#).

Parameters

`assert_insample_perf` logical(1)

Should the insample performance of the [mlr3::LearnerRegr](#) be asserted after updating the surrogate? If the assertion fails (i.e., the insample performance based on the `perf_measure` does not meet the `perf_threshold`), an error is thrown. Default is FALSE.

`perf_measure` [mlr3::MeasureRegr](#)

Performance measure which should be use to assert the insample performance of the [mlr3::LearnerRegr](#). Only relevant if `assert_insample_perf = TRUE`. Default is [mlr3::mlr_measures_regr.rsq](#).

`perf_threshold` numeric(1)

Threshold the insample performance of the [mlr3::LearnerRegr](#) should be asserted against. Only relevant if `assert_insample_perf = TRUE`. Default is 0.

`catch_errors` logical(1)

Should errors during updating the surrogate be caught and propagated to the `loop_function` which can then handle the failed infill optimization (as a result of the failed surrogate) appropriately by, e.g., proposing a randomly sampled point for evaluation? Default is TRUE.

Super class

[mlr3mbo::Surrogate](#) -> SurrogateLearner

Active bindings

- `print_id` (character)
Id used when printing.
- `n_learner` (integer(1))
Returns the number of surrogate models.
- `assert_insample_perf` (numeric())
Asserts whether the current insample performance meets the performance threshold.
- `packages` (character())
Set of required packages. A warning is signaled if at least one of the packages is not installed, but loaded (not attached) later on-demand via [requireNamespace\(\)](#).
- `feature_types` (character())
Stores the feature types the surrogate can handle, e.g. "logical", "numeric", or "factor". A complete list of candidate feature types, grouped by task type, is stored in [mlr_reflections\\$task_feature_types](#).
- `properties` (character())
Stores a set of properties/capabilities the surrogate has. A complete list of candidate properties, grouped by task type, is stored in [mlr_reflections\\$learner_properties](#).
- `predict_type` (character(1))
Retrieves the currently active predict type, e.g. "response".

Methods**Public methods:**

- [SurrogateLearner\\$new\(\)](#)
- [SurrogateLearner\\$predict\(\)](#)
- [SurrogateLearner\\$clone\(\)](#)

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

Usage:

`SurrogateLearner$new(learner, archive = NULL, x_cols = NULL, y_col = NULL)`

Arguments:

`learner` ([mlr3::LearnerRegr](#)).

`archive` ([bbotk::Archive](#) | NULL)

[bbotk::Archive](#) of the [bbotk::OptimInstance](#).

`x_cols` (character() | NULL)

Column Id's of variables that should be used as features. By default, automatically inferred based on the archive.

`y_col` (character(1) | NULL)

Column Id of variable that should be used as a target. By default, automatically inferred based on the archive.

Method `predict()`: Predict mean response and standard error.

Usage:

`SurrogateLearner$predict(xdt)`

Arguments:

```
xdt (data.table::data.table())
  New data. One row per observation.
```

Returns: `data.table::data.table()` with the columns mean and se.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Examples

```
if (requireNamespace("mlr3learners") &
    requireNamespace("DiceKriging") &
    requireNamespace("rgenoud")) {
  library(bbotk)
  library(paradox)
  library(mlr3learners)

  fun = function(xs) {
    list(y = xs$x ^ 2)
  }
  domain = ps(x = p_dbl(lower = -10, upper = 10))
  codomain = ps(y = p_dbl(tags = "minimize"))
  objective = ObjectiveRfun$new(fun = fun, domain = domain, codomain = codomain)

  instance = OptimInstanceSingleCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))

  xdt = generate_design_random(instance$search_space, n = 4)$data

  instance$eval_batch(xdt)

  learner = lrn("regr.km",
    covtype = "matern3_2",
    optim.method = "gen",
    nugget.stability = 10^-8,
    control = list(trace = FALSE))

  surrogate = srlrn(learner, archive = instance$archive)

  surrogate$update()

  surrogate$model$model
}
```

 SurrogateLearnerCollection

Surrogate Model Containing Multiple Learners

Description

Surrogate model containing multiple [mlr3::LearnerRegr](#). The [mlr3::LearnerRegr](#) are fit on the target variables as indicated via `y_cols`. Note that redundant [mlr3::LearnerRegr](#) must be deep clones.

Parameters

`assert_insample_perf` `logical(1)`

Should the insample performance of the [mlr3::LearnerRegr](#) be asserted after updating the surrogate? If the assertion fails (i.e., the insample performance based on the `perf_measure` does not meet the `perf_threshold`), an error is thrown. Default is FALSE.

`perf_measure` List of [mlr3::MeasureRegr](#)

Performance measures which should be used to assert the insample performance of the [mlr3::LearnerRegr](#). Only relevant if `assert_insample_perf = TRUE`. Default is [mlr3::mlr_measures_regr.rsq](#) for each learner.

`perf_threshold` List of `numeric(1)`

Thresholds the insample performance of the [mlr3::LearnerRegr](#) should be asserted against. Only relevant if `assert_insample_perf = TRUE`. Default is 0 for each learner.

`catch_errors` `logical(1)`

Should errors during updating the surrogate be caught and propagated to the `loop_function` which can then handle the failed infill optimization (as a result of the failed surrogate) appropriately by, e.g., proposing a randomly sampled point for evaluation? Default is TRUE.

Super class

[mlr3mbo::Surrogate](#) -> SurrogateLearnerCollection

Active bindings

`print_id` (`character`)

Id used when printing.

`n_learner` (`integer(1)`)

Returns the number of surrogate models.

`assert_insample_perf` (`numeric()`)

Asserts whether the current insample performance meets the performance threshold.

`packages` (`character()`)

Set of required packages. A warning is signaled if at least one of the packages is not installed, but loaded (not attached) later on-demand via [requireNamespace\(\)](#).

`feature_types` (`character()`)

Stores the feature types the surrogate can handle, e.g. "logical", "numeric", or "factor". A complete list of candidate feature types, grouped by task type, is stored in [mlr_reflections\\$task_feature_types](#).

`properties` (character())
Stores a set of properties/capabilities the surrogate has. A complete list of candidate properties, grouped by task type, is stored in `mlr_reflections$learner_properties`.

`predict_type` (character(1))
Retrieves the currently active predict type, e.g. "response".

Methods

Public methods:

- [SurrogateLearnerCollection\\$new\(\)](#)
- [SurrogateLearnerCollection\\$predict\(\)](#)
- [SurrogateLearnerCollection\\$clone\(\)](#)

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

Usage:

```
SurrogateLearnerCollection$new(
  learners,
  archive = NULL,
  x_cols = NULL,
  y_cols = NULL
)
```

Arguments:

`learners` (list of [mlr3::LearnerRegr](#)).

`archive` ([bbotk::Archive](#) | NULL)
[bbotk::Archive](#) of the [bbotk::OptimInstance](#).

`x_cols` (character() | NULL)
Column Id's of variables that should be used as features. By default, automatically inferred based on the archive.

`y_cols` (character() | NULL)
Column Id's of variables that should be used as targets. By default, automatically inferred based on the archive.

Method `predict()`: Predict mean response and standard error. Returns a named list of `data.tables`. Each contains the mean response and standard error for one `y_col`.

Usage:

```
SurrogateLearnerCollection$predict(xdt)
```

Arguments:

`xdt` ([data.table::data.table\(\)](#))
New data. One row per observation.

Returns: list of [data.table::data.table\(\)](#)s with the columns `mean` and `se`.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Examples

```

if (requireNamespace("mlr3learners") &
    requireNamespace("DiceKriging") &
    requireNamespace("rgenoud") &
    requireNamespace("ranger")) {
  library(bbotk)
  library(paradox)
  library(mlr3learners)

  fun = function(xs) {
    list(y1 = xs$x^2, y2 = (xs$x - 2) ^ 2)
  }
  domain = ps(x = p_dbl(lower = -10, upper = 10))
  codomain = ps(y1 = p_dbl(tags = "minimize"), y2 = p_dbl(tags = "minimize"))
  objective = ObjectiveRfun$new(fun = fun, domain = domain, codomain = codomain)

  instance = OptimInstanceMultiCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))
  xdt = generate_design_random(instance$search_space, n = 4)$data

  instance$eval_batch(xdt)

  learner1 = lrn("regr.km",
    covtype = "matern3_2",
    optim.method = "gen",
    nugget.stability = 10^-8,
    control = list(trace = FALSE))

  learner2 = lrn("regr.ranger",
    num.trees = 500,
    keep.inbag = TRUE,
    se.method = "jack")

  surrogate = srlrnc(list(learner1, learner2), archive = instance$archive)

  surrogate$update()

  surrogate$model

  surrogate$model[["y2"]$model
}

```

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