Package 'mlr3mbo'

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Type Package

Title Flexible Bayesian Optimization

Version 0.2.6

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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URL https://mlr3mbo.mlr-org.com, https://github.com/mlr-org/mlr3mbo

BugReports https://github.com/mlr-org/mlr3mbo/issues

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'AcqFunctionCB.R' 'AcqFunctionEHVI.R' 'AcqFunctionEHVIGH.R'
'AcqFunctionEI.R' 'AcqFunctionEIPS.R' 'AcqFunctionMean.R'
'AcqFunctionMulti.R' 'AcqFunctionPI.R' 'AcqFunctionSD.R'
'AcqFunctionSmsEgo.R' 'AcqOptimizer.R' 'aaa.R' 'OptimizerMbo.R'
'mlr_result_assigners.R' 'ResultAssigner.R'
'ResultAssignerArchive.R' 'ResultAssignerSurrogate.R'
'Surrogate.R' 'SurrogateLearner.R'
'SurrogateLearnerCollection.R' 'TunerMbo.R'
'mlr_loop_functions.R' 'bayesopt_ego.R' 'bayesopt_emo.R'
'bayesopt_mpcl.R' 'bayesopt_parego.R' 'bayesopt_smsego.R'
'bibentries.R' 'helper.R' 'loop_function.R' 'mbo_defaults.R'
'sugar.R' 'zzz.R'

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Contents

`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, ParEGO by Knowles (2006) doi:10.1109/TEVC.2005.851274 and SMS-EGO by Ponweiser et al. (2008) doi: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

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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

`.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.

Value

AcqFunction

Examples

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

---

acqfs *Syntactic Sugar Acquisition Functions Construction*

Description

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

Usage

```
acqfs(.keys, ...)
```

Arguments

`.keys`	(`character()`) Keys passed to the respective dictionary to retrieve multiple objects.
`...`	(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

List of AcqFunctions

Examples

```
acqfs(c("ei", "pi", "cb"))
```

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`)
: Points 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`.

`packages` (`character()`)
: Set of required packages.

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,
  packages = NULL,
  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"`.

`packages` (`character()`)
Set of required packages. A warning is signaled prior to construction if at least one of the packages is not installed, but loaded (not attached) later on-demand via `requireNamespace()`.

`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, mlr_acqfunctions_aei, mlr_acqfunctions_cb, mlr_acqfunctions_ehvi, mlr_acqfunctions_ehvigh, mlr_acqfunctions_ei, mlr_acqfunctions_eips, mlr_acqfunctions_mean, mlr_acqfunctions_multi, mlr_acqfunctions_pi, mlr_acqfunctions_sd, mlr_acqfunctions_smsego

---

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, callbacks = NULL, ...)
```

Arguments

`optimizer`	(bbotk::Optimizer) bbotk::Optimizer that is to be used.
`terminator`	(bbotk::Terminator) bbotk::Terminator that is to be used.
`acq_function`	(`NULL` | AcqFunction) AcqFunction that is to be used. Can also be `NULL`.
`callbacks`	(`NULL` | list of mlr3misc::Callback) Callbacks used during acquisition function optimization.
`...`	(named `list()`) 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 acquisition function optimization. Wraps an bbotk::Optimizer and bbotk::Terminator.

Parameters

`n_candidates integer(1)`
: Number of candidate points to propose. Note that this does not affect how the acquisition function itself is calculated (e.g., setting `n_candidates > 1` will not result in computing the q- or multi-Expected Improvement) but rather the top `n_candidates` are selected from the bbotk::Archive of the acquisition function bbotk::OptimInstance. Note that setting `n_candidates > 1` is usually not a sensible idea but it is still supported for experimental reasons. Note that in the case of the acquisition function bbotk::OptimInstance being multi-criteria, due to using an AcqFunctionMulti, selection of the best candidates is performed via non-dominated-sorting. Default is `1`.

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

`warmstart logical(1)`
: Should the acquisition function optimization be warm-started by evaluating the best point(s) present in the bbotk::Archive of the actual bbotk::OptimInstance (which is contained in the archive of the AcqFunction)? This is sensible when using a population based acquisition function optimizer, e.g., local search or mutation. Default is `FALSE`. Note that in the case of the bbotk::OptimInstance being multi-criteria, selection of the best point(s) is performed via non-dominated-sorting.

`warmstart_size integer(1) | "all"`
: Number of best points selected from the bbotk::Archive of the actual bbotk::OptimInstance that are to be used for warm starting. Can either be an integer or "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(s) resulting of the acquisition function optimization were already evaluated on the actual bbotk::OptimInstance. Should such candidate proposals be ignored and only candidates that were yet not evaluated be considered? Default is `TRUE`.

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

Public fields

`optimizer` (bbotk::Optimizer).

`terminator` (bbotk::Terminator).

`acq_function` (AcqFunction).

`callbacks` (`NULL` | list of mlr3misc::Callback).

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, callbacks = NULL)
```

Arguments:

`optimizer` (bbotk::Optimizer).

`terminator` (bbotk::Terminator).

`acq_function` (`NULL` | AcqFunction).

`callbacks` (`NULL` | list of mlr3misc::Callback)

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

Usage:

```
AcqOptimizer$format()
```

Returns: (`character(1)`).

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 candidate.

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.

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

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

  learner = default_gp()

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

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

  acq_function$surrogate$update()
  acq_function$update()

  acq_optimizer = acqo(
    optimizer = opt("random_search", batch_size = 1000),
    terminator = trm("evals", n_evals = 1000),
    acq_function = acq_function)
```

```
  acq_optimizer$optimize()
}
```

`default_acqfunction` *Default Acquisition Function*

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_acqfunction(instance)
```

Arguments

`instance`	(bbotk::OptimInstance).

Value

AcqFunction

See Also

Other mbo_defaults: `default_acqoptimizer()`, `default_gp()`, `default_loop_function()`, `default_result_assigner`
`default_rf()`, `default_surrogate()`, `mbo_defaults`

`default_acqoptimizer` *Default Acquisition Function Optimizer*

Description

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

Usage

```
default_acqoptimizer(acq_function)
```

Arguments

`acq_function`	(AcqFunction).

Value

AcqOptimizer

See Also

Other mbo_defaults: default_acqfunction(), default_gp(), default_loop_function(), default_result_assigner(), default_rf(), default_surrogate(), mbo_defaults

---

`default_gp` *Default Gaussian Process*

Description

This is a helper function that constructs a default Gaussian Process mlr3::LearnerRegr which is for example used in default_surrogate.

Constructs a Kriging learner ""regr.km"" with kernel ""matern5_2"". If `noisy = FALSE` (default) a small nugget effect is added `nugget.stability = 10^-8` to increase numerical stability to hopefully prevent crashes of **DiceKriging**. If `noisy = TRUE` the nugget effect will be estimated with `nugget.estim = TRUE`. If `noisy = TRUE` `jitter` is set to `TRUE` to circumvent a problem with **DiceKriging** where already trained input values produce the exact trained output. In general, 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 model prediction.

Usage

```
default_gp(noisy = FALSE)
```

Arguments

`noisy`	(logical(1)) Whether the learner will be used in a noisy objective function scenario. See above.

Value

mlr3::LearnerRegr

See Also

Other mbo_defaults: default_acqfunction(), default_acqoptimizer(), default_loop_function(), default_result_assigner(), default_rf(), default_surrogate(), mbo_defaults

default_loop_function *Default Loop Function*

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_loop_function(instance)
```

Arguments

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

Value

loop_function

See Also

Other mbo_defaults: `default_acqfunction()`, `default_acqoptimizer()`, `default_gp()`, `default_result_assigner()`, `default_rf()`, `default_surrogate()`, `mbo_defaults`

default_result_assigner *Default Result Assigner*

Description

Chooses a default result assigner. Defaults to ResultAssignerArchive.

Usage

```
default_result_assigner(instance)
```

Arguments

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

Value

ResultAssigner

See Also

Other mbo_defaults: default_acqfunction(), default_acqoptimizer(), default_gp(), default_loop_function(), default_rf(), default_surrogate(), mbo_defaults

---

`default_rf` *Default Random Forest*

Description

This is a helper function that constructs a default random forest mlr3::LearnerRegr which is for example used in default_surrogate.

Constructs a ranger learner ""regr.ranger"" with `num.trees` = `100`, `keep.inbag` = `TRUE` and `se.method` = `"jack"`.

Usage

```
default_rf(noisy = FALSE)
```

Arguments

`noisy`	(logical(1)) Whether the learner will be used in a noisy objective function scenario. Currently has no effect.

Value

mlr3::LearnerRegr

See Also

Other mbo_defaults: default_acqfunction(), default_acqoptimizer(), default_gp(), default_loop_function(), default_result_assigner(), default_surrogate(), mbo_defaults

---

`default_surrogate` *Default Surrogate*

Description

This is a helper function that constructs a default Surrogate based on properties of the bbotk::OptimInstance.

For numeric-only (including integers) parameter spaces without any dependencies a Gaussian Process is constricted via `default_gp()`. For mixed numeric-categorical parameter spaces, or spaces with conditional parameters a random forest is constructed via `default_rf()`.

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 = 10L, 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 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::OptimInstanceBatchSingleCrit the learner is wrapped as a SurrogateLearner.

If the instance is of class bbotk::OptimInstanceBatchMultiCrit multiple deep clones of the learner are wrapped as a SurrogateLearnerCollection.

Usage

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

Arguments

`instance`	(bbotk::OptimInstance) An object that inherits from bbotk::OptimInstance.
`learner`	(`NULL` | mlr3::Learner). If specified, this learner will be used instead of the defaults described above.
`n_learner`	(`NULL` | `integer(1)`). Number of learners to be considered in the construction of the SurrogateLearner or SurrogateLearnerCollection. If not specified will be based on the number of objectives as stated by the instance.

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_acqfunction(), default_acqoptimizer(), default_gp(), default_loop_function(), default_result_assigner(), default_rf(), mbo_defaults

---

`loop_function` *Loop Functions for Bayesian Optimization*

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, mlr_loop_functions_ego, mlr_loop_functions_emo, mlr_loop_functions_mpcl, mlr_loop_functions_parego, mlr_loop_functions_smsego

---

`mbo_defaults` *Defaults for OptimizerMbo*

Description

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

- Optimization Loop: default_loop_function
- Surrogate: default_surrogate
- Acquisition Function: default_acqfunction
- Acqfun Optimizer: default_acqoptimizer
- Result Assigner: default_result_assigner

See Also

Other mbo_defaults: default_acqfunction(), default_acqoptimizer(), default_gp(), default_loop_function(), default_result_assigner(), default_rf(), 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()` and `acqfs()`.

Format

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

Methods

See mlr3misc::Dictionary.

See Also

Sugar functions: `acqf()`, `acqfs()`

Other Dictionary: `mlr_loop_functions`, `mlr_result_assigners`

Other Acquisition Function: `AcqFunction`, `mlr_acqfunctions_aei`, `mlr_acqfunctions_cb`, `mlr_acqfunctions_ehvi`, `mlr_acqfunctions_ehvigh`, `mlr_acqfunctions_ei`, `mlr_acqfunctions_eips`, `mlr_acqfunctions_mean`, `mlr_acqfunctions_multi`, `mlr_acqfunctions_pi`, `mlr_acqfunctions_sd`, `mlr_acqfunctions_smsego`

Examples

```
library(data.table)
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(): Update the acquisition function and set 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, mlr_acqfunctions_cb, mlr_acqfunctions_ehvi, mlr_acqfunctions_ehvigh, mlr_acqfunctions_ei, mlr_acqfunctions_eips, mlr_acqfunctions_mean, mlr_acqfunctions_multi, mlr_acqfunctions_pi, mlr_acqfunctions_sd, mlr_acqfunctions_smsego

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 = OptimInstanceBatchSingleCrit$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 = "matern5_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, mlr_acqfunctions_aei, mlr_acqfunctions_ehvi, mlr_acqfunctions_ehvigh, mlr_acqfunctions_ei, mlr_acqfunctions_eips, mlr_acqfunctions_mean, mlr_acqfunctions_multi, mlr_acqfunctions_pi, mlr_acqfunctions_sd, mlr_acqfunctions_smsego

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

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

  learner = default_gp()

  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_ehvi *Acquisition Function Expected Hypervolume Improvement*

Description

Exact Expected Hypervolume Improvement. Calculates the exact expected hypervolume improvement in the case of two objectives. In the case of optimizing more than two objective functions, AcqFunctionEHVIGH can be used. See Emmerich et al. (2016) for details.

Super classes

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

Public fields

`ys_front` (`matrix()`)
: Approximated Pareto front. Sorted by the first objective. Signs are corrected with respect to assuming minimization of objectives.

`ref_point` (`numeric()`)
: Reference point. Signs are corrected with respect to assuming minimization of objectives.

`ys_front_augmented` (`matrix()`)
: Augmented approximated Pareto front. Sorted by the first objective. Signs are corrected with respect to assuming minimization of objectives.

Methods

Public methods:

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

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

Usage:

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

Arguments:

`surrogate` (`NULL` | SurrogateLearnerCollection).

Method `update()`**:** Update the acquisition function and set `ys_front` and `ref_point`.

Usage:

```
AcqFunctionEHVI$update()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

References

- Emmerich, Michael, Yang, Kaifeng, Deutz, André, Wang, Hao, Fonseca, M. C (2016). "A Multicriteria Generalization of Bayesian Global Optimization." In Pardalos, M. P, Zhigljavsky, Anatoly, Žilinskas, Julius (eds.), *Advances in Stochastic and Deterministic Global Optimization*, 229–242. Springer International Publishing, Cham.

See Also

Other Acquisition Function: AcqFunction, mlr_acqfunctions, mlr_acqfunctions_aei, mlr_acqfunctions_cb, mlr_acqfunctions_ehvigh, mlr_acqfunctions_ei, mlr_acqfunctions_eips, mlr_acqfunctions_mean, mlr_acqfunctions_multi, mlr_acqfunctions_pi, mlr_acqfunctions_sd, mlr_acqfunctions_smsego

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

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

  learner = default_gp()

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

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

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

---

mlr_acqfunctions_ehvigh

Acquisition Function Expected Hypervolume Improvement via Gauss-Hermite Quadrature

---

Description

Expected Hypervolume Improvement. Computed via Gauss-Hermite quadrature.

In the case of optimizing only two objective functions AcqFunctionEHVI is to be preferred.

Parameters

- `"k"` (`integer(1)`)
  Number of nodes per objective used for the numerical integration via Gauss-Hermite quadrature. Defaults to 15. For example, if two objectives are to be optimized, the total number of nodes will therefore be 225 per default. Changing this value after construction requires a call to `$update()` to update the `$gh_data` field.
- `"r"` (`numeric(1)`)
  Pruning rate between 0 and 1 that determines the fraction of nodes of the Gauss-Hermite quadrature rule that are ignored based on their weight value (the nodes with the lowest weights being ignored). Default is `0.2`. Changing this value after construction does not require a call to `$update()`.

Super classes

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

Public fields

`ys_front` (`matrix()`)
: Approximated Pareto front. Signs are corrected with respect to assuming minimization of objectives.

`ref_point` (`numeric()`)
: Reference point. Signs are corrected with respect to assuming minimization of objectives.

`hypervolume` (`numeric(1)`). Current hypervolume of the approximated Pareto front with respect to the reference point.

`gh_data` (`matrix()`)
: Data required for the Gauss-Hermite quadrature rule in the form of a matrix of dimension (k x 2). Each row corresponds to one Gauss-Hermite node (column `"x"`) and corresponding weight (column `"w"`). Computed via fastGHQuad::gaussHermiteData. Nodes are scaled by a factor of `sqrt(2)` and weights are normalized under a sum to one constraint.

Methods

Public methods:

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

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

Usage:

```
AcqFunctionEHVIGH$new(surrogate = NULL, k = 15L, r = 0.2)
```

Arguments:

`surrogate` (`NULL` | SurrogateLearnerCollection).

`k` (`integer(1)`).

`r` (`numeric(1)`).

Method `update()`**:** Update the acquisition function and set `ys_front`, `ref_point`, `hypervolume` and `gh_data`.

Usage:

```
AcqFunctionEHVIGH$update()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

References

- Rahat, Alma, Chugh, Tinkle, Fieldsend, Jonathan, Allmendinger, Richard, Miettinen, Kaisa (2022). "Efficient Approximation of Expected Hypervolume Improvement using Gauss-Hermit Quadrature." In Rudolph, Günter, Kononova, V. A, Aguirre, Hernán, Kerschke, Pascal, Ochoa, Gabriela, Tušar, Tea (eds.), *Parallel Problem Solving from Nature – PPSN XVII*, 90–103.

See Also

Other Acquisition Function: AcqFunction, mlr_acqfunctions, mlr_acqfunctions_aei, mlr_acqfunctions_cb, mlr_acqfunctions_ehvi, mlr_acqfunctions_ei, mlr_acqfunctions_eips, mlr_acqfunctions_mean, mlr_acqfunctions_multi, mlr_acqfunctions_pi, mlr_acqfunctions_sd, mlr_acqfunctions_smsego

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 = OptimInstanceBatchMultiCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))
```

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

  learner = default_gp()

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

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

  acq_function$surrogate$update()
  acq_function$update()
  acq_function$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")
```

Parameters

- `"epsilon"` (`numeric(1)`)
  ϵ value used to determine the amount of exploration. Higher values result in the importance of improvements predicted by the posterior mean decreasing relative to the importance of potential improvements in regions of high predictive uncertainty. Defaults to `0` (standard Expected Improvement).

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, epsilon = 0)
```

Arguments:

`surrogate` (`NULL` | SurrogateLearner).

`epsilon` (`numeric(1)`).

Method `update()`**:** Update the acquisition function and set `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, mlr_acqfunctions_aei, mlr_acqfunctions_cb, mlr_acqfunctions_ehvi, mlr_acqfunctions_ehvigh, mlr_acqfunctions_eips, mlr_acqfunctions_mean, mlr_acqfunctions_multi, mlr_acqfunctions_pi, mlr_acqfunctions_sd, mlr_acqfunctions_smsego

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

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

  learner = default_gp()

  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::OptimInstanceBatchSingleCrit. Additionally to target values of the codomain that should be minimized or maximized, the bbotk::Objective of the bbotk::OptimInstanceBatchSingleCrit should return time values. The column names of the target variable and time variable must be passed as `cols_y` 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

`col_y` (`character(1)`).

`col_time` (`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()`**:** Update the acquisition function and set `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`, `mlr_acqfunctions_aei`, `mlr_acqfunctions_cb`, `mlr_acqfunctions_ehvi`, `mlr_acqfunctions_ehvigh`, `mlr_acqfunctions_ei`, `mlr_acqfunctions_mean`, `mlr_acqfunctions_multi`, `mlr_acqfunctions_pi`, `mlr_acqfunctions_sd`, `mlr_acqfunctions_smsego`

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

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

  learner = default_gp()

 surrogate = srlrn(list(learner, learner$clone(deep = TRUE)), archive = instance$archive)
  surrogate$cols_y = 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, mlr_acqfunctions_aei, mlr_acqfunctions_cb, mlr_acqfunctions_ehvi, mlr_acqfunctions_ehvigh, mlr_acqfunctions_ei, mlr_acqfunctions_eips, mlr_acqfunctions_multi, mlr_acqfunctions_pi, mlr_acqfunctions_sd, mlr_acqfunctions_smsego

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

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

  learner = default_gp()
```

```
  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_multi` *Acquisition Function Wrapping Multiple Acquisition Functions*

Description

Wrapping multiple AcqFunctions resulting in a multi-objective acquisition function composed of the individual ones. Note that the optimization direction of each wrapped acquisition function is corrected for maximization.

For each acquisition function, the same Surrogate must be used. If acquisition functions passed during construction already have been initialized with a surrogate, it is checked whether the surrogate is the same for all acquisition functions. If acquisition functions have not been initialized with a surrogate, the surrogate passed during construction or lazy initialization will be used for all acquisition functions.

For optimization, AcqOptimizer can be used as for any other AcqFunction, however, the bbotk::Optimizer wrapped within the AcqOptimizer must support multi-objective optimization as indicated via the `multi-crit` property.

Dictionary

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

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

Super classes

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

Active bindings

`surrogate` (Surrogate)
: Surrogate.

`acq_functions` (list of AcqFunction)
: Points to the list of the individual acquisition functions.

`acq_function_ids` (character())
: Points to the ids of the individual acquisition functions.

Methods

Public methods:

- AcqFunctionMulti$new()
- AcqFunctionMulti$update()
- AcqFunctionMulti$clone()

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

Usage:

```
AcqFunctionMulti$new(acq_functions, surrogate = NULL)
```

Arguments:

`acq_functions` (list of AcqFunctions).

`surrogate` (`NULL` | Surrogate).

Method `update()`**:** Update each of the wrapped acquisition functions.

Usage:

```
AcqFunctionMulti$update()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

See Also

Other Acquisition Function: AcqFunction, mlr_acqfunctions, mlr_acqfunctions_aei, mlr_acqfunctions_cb, mlr_acqfunctions_ehvi, mlr_acqfunctions_ehvigh, mlr_acqfunctions_ei, mlr_acqfunctions_eips, mlr_acqfunctions_mean, mlr_acqfunctions_pi, mlr_acqfunctions_sd, mlr_acqfunctions_smsego

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 = OptimInstanceBatchSingleCrit$new(
```

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

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

  learner = default_gp()

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

  acq_function = acqf("multi",
    acq_functions = acqfs(c("ei", "pi", "cb")),
    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()`**:** Update the acquisition function and set `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 Multipeak Curve in the Presence of Noise." *Journal of Basic Engineering*, **86**(1), 97–106.

See Also

Other Acquisition Function: `AcqFunction`, `mlr_acqfunctions`, `mlr_acqfunctions_aei`, `mlr_acqfunctions_cb`, `mlr_acqfunctions_ehvi`, `mlr_acqfunctions_ehvigh`, `mlr_acqfunctions_ei`, `mlr_acqfunctions_eips`, `mlr_acqfunctions_mean`, `mlr_acqfunctions_multi`, `mlr_acqfunctions_sd`, `mlr_acqfunctions_smsego`

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

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

  learner = default_gp()

  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_sd` *Acquisition Function Standard Deviation*

Description

Posterior Standard Deviation.

Dictionary

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

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

Super classes

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

Methods

Public methods:

- `AcqFunctionSD$new()`
- `AcqFunctionSD$clone()`

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

Usage:

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

Arguments:

`surrogate` (`NULL` | SurrogateLearner).

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

See Also

Other Acquisition Function: AcqFunction, mlr_acqfunctions, mlr_acqfunctions_aei, mlr_acqfunctions_cb, mlr_acqfunctions_ehvi, mlr_acqfunctions_ehvigh, mlr_acqfunctions_ei, mlr_acqfunctions_eips, mlr_acqfunctions_mean, mlr_acqfunctions_multi, mlr_acqfunctions_pi, mlr_acqfunctions_smsego

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

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

  learner = default_gp()

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

  acq_function = acqf("sd", 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 `confidence = (1 - 2 * 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. Signs are corrected with respect to assuming minimization of objectives.

`ref_point` (`numeric()`)
Reference point. Signs are corrected with respect to assuming minimization of objectives.

`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()`**:** Update the acquisition function and set `ys_front`, `ref_point` and `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, mlr_acqfunctions_aei, mlr_acqfunctions_cb, mlr_acqfunctions_ehvi, mlr_acqfunctions_ehvigh, mlr_acqfunctions_ei, mlr_acqfunctions_eips, mlr_acqfunctions_mean, mlr_acqfunctions_multi, mlr_acqfunctions_pi, mlr_acqfunctions_sd

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

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

  learner = default_gp()

  surrogate = srlrn(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

`key`	(`character(1)`).
`...`	(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, mlr_result_assigners

Other Loop Function: loop_function, mlr_loop_functions_ego, mlr_loop_functions_emo, mlr_loop_functions_mpcl, mlr_loop_functions_parego, mlr_loop_functions_smsego

Examples

```
library(data.table)
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,
  surrogate,
  acq_function,
  acq_optimizer,
  init_design_size = NULL,
  random_interleave_iter = 0L
)
```

Arguments

instance	(bbotk::OptimInstanceBatchSingleCrit) The bbotk::OptimInstanceBatchSingleCrit to be optimized.
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.

`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 generated via a Sobol sequence.

`random_interleave_iter`
: (`integer(1)`)
Every `random_interleave_iter` iteration (starting after the initial design), a point is sampled uniformly at random and evaluated (instead of a model based proposal). For example, if `random_interleave_iter = 2`, 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::OptimInstanceBatchSingleCrit.

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`, `mlr_loop_functions_emo`, `mlr_loop_functions_mpcl`, `mlr_loop_functions_parego`, `mlr_loop_functions_smsego`

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

  surrogate = default_surrogate(instance, n_learner = 2)
  surrogate$cols_y = 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_emo` *Sequential Multi-Objective Bayesian Optimization*

Description

Loop function for sequential multi-objective Bayesian Optimization. Normally used inside an OptimizerMbo. The conceptual counterpart to mlr_loop_functions_ego.

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

Arguments

`instance`	(bbotk::OptimInstanceBatchMultiCrit) The bbotk::OptimInstanceBatchMultiCrit to be optimized.
`surrogate`	(SurrogateLearnerCollection) SurrogateLearnerCollection 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.
`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 generated via a Sobol sequence.
`random_interleave_iter`	(`integer(1)`) Every `random_interleave_iter` iteration (starting after the initial design), a point is sampled uniformly at random and evaluated (instead of a model based proposal). For example, if `random_interleave_iter = 2`, 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::OptimInstanceBatchMultiCrit.

See Also

Other Loop Function: `loop_function`, `mlr_loop_functions`, `mlr_loop_functions_ego`, `mlr_loop_functions_mpcl`, `mlr_loop_functions_parego`, `mlr_loop_functions_smsego`

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

  surrogate = default_surrogate(instance)

  acq_function = acqf("ehvi")

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

  optimizer = opt("mbo",
    loop_function = bayesopt_emo,
    surrogate = surrogate,
    acq_function = acq_function,
```

```
    acq_optimizer = acq_optimizer)

  optimizer$optimize(instance)
}
```

`mlr_loop_functions_mpcl` *Single-Objective Bayesian Optimization via Multipoint Constant Liar*

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

Arguments

`instance`	(bbotk::OptimInstanceBatchSingleCrit) The bbotk::OptimInstanceBatchSingleCrit to be optimized.
`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.

`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 generated via a Sobol sequence.

`q` (`integer(1)`)
Batch size > 1. Default is 2.

`liar` (`function`)
Any function accepting a numeric vector as input and returning a single numeric output. Default is `mean`. Other sensible functions include `min` (or `max`, depending on the optimization direction).

`random_interleave_iter`
(`integer(1)`)
Every `random_interleave_iter` iteration (starting after the initial design), a point is sampled uniformly at random and evaluated (instead of a model based proposal). For example, if `random_interleave_iter = 2`, 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::OptimInstanceBatchSingleCrit.
- To make use of parallel evaluations in the case of 'q > 1, the objective function of the bbotk::OptimInstanceBatchSingleC 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`, `mlr_loop_functions_ego`, `mlr_loop_functions_emo`, `mlr_loop_functions_parego`, `mlr_loop_functions_smsego`

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 = OptimInstanceBatchSingleCrit$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,
  surrogate,
  acq_function,
  acq_optimizer,
  init_design_size = NULL,
  q = 1L,
  s = 100L,
  rho = 0.05,
  random_interleave_iter = 0L
)
```

Arguments

`instance`	(bbotk::OptimInstanceBatchMultiCrit) The bbotk::OptimInstanceBatchMultiCrit to be optimized.
`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.
`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 generated via a Sobol sequence.
`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 `random_interleave_iter` iteration (starting after the initial design), a point is sampled uniformly at random and evaluated (instead of a model based proposal). For example, if `random_interleave_iter = 2`, 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::OptimInstanceBatchMultiCrit.
- The scalarizations of the objective function values are stored as the `y_scal` column in the bbotk::Archive of the bbotk::OptimInstanceBatchMultiCrit.
- To make use of parallel evaluations in the case of 'q > 1, the objective function of the bbotk::OptimInstanceBatchMultiCr 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`, `mlr_loop_functions_ego`, `mlr_loop_functions_emo`, `mlr_loop_functions_mpcl`, `mlr_loop_functions_smsego`

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 = OptimInstanceBatchMultiCrit$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,
  surrogate,
  acq_function,
  acq_optimizer,
  init_design_size = NULL,
  random_interleave_iter = 0L
)
```

Arguments

`instance`	(bbotk::OptimInstanceBatchMultiCrit) The bbotk::OptimInstanceBatchMultiCrit to be optimized.
`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.

`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 generated via a Sobol sequence.

`random_interleave_iter`
(`integer(1)`)
Every `random_interleave_iter` iteration (starting after the initial design), a point is sampled uniformly at random and evaluated (instead of a model based proposal). For example, if `random_interleave_iter = 2`, 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::OptimInstanceBatchMultiCrit.
- Due to the iterative computation of the epsilon within the mlr_acqfunctions_smsego, requires the bbotk::Terminator of the bbotk::OptimInstanceBatchMultiCrit 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`, `mlr_loop_functions_ego`, `mlr_loop_functions_emo`, `mlr_loop_functions_mpcl`, `mlr_loop_functions_parego`

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 = OptimInstanceBatchMultiCrit$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.

Note that in general the Surrogate is updated one final time on all available data after the optimization process has terminated. However, in certain scenarios this is not always possible or meaningful, e.g., when using `bayesopt_parego()` for multi-objective optimization which uses a surrogate that relies on a scalarization of the objectives. It is therefore recommended to manually inspect the Surrogate after optimization if it is to be used, e.g., for visualization purposes to make sure that it has been properly updated on all available data. If this final update of the Surrogate could not be performed successfully, a warning will be logged.

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 classes

`bbotk::Optimizer` -> `bbotk::OptimizerBatch` -> `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_assigner` (ResultAssigner | `NULL`)
: The result assigner.

`param_classes` (`character()`)
: Supported parameter classes that the optimizer can optimize. Determined based on the `surrogate` and the `acq_optimizer`. This corresponds to the values given by a paradox::ParamSet's `$class` field.

`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 acq_function, 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_acqfunction(instance) is used. If acq_optimizer is NULL, default_acqoptimizer(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_assigner = 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_assigner (ResultAssigner | NULL)
: The result assigner.

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_assigner`

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 = OptimInstanceBatchSingleCrit$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)

# 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 = OptimInstanceBatchMultiCrit$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_result_assigners` *Dictionary of Result Assigners*

Description

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

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

Format

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

Methods

See mlr3misc::Dictionary.

See Also

Sugar function: `ras()`

Other Dictionary: `mlr_acqfunctions`, `mlr_loop_functions`

Other Result Assigner: `ResultAssigner`, `mlr_result_assigners_archive`, `mlr_result_assigners_surrogate`

Examples

```
library(data.table)
as.data.table(mlr_result_assigners)
ras("archive")
```

`mlr_result_assigners_archive`

Result Assigner Based on the Archive

Description

Result assigner that chooses the final point(s) based on all evaluations in the bbotk::Archive. This mimics the default behavior of any bbotk::Optimizer.

Super class

`mlr3mbo::ResultAssigner` -> `ResultAssignerArchive`

Active bindings

`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()`.

Methods

Public methods:

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

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

Usage:

```
ResultAssignerArchive$new()
```

Method `assign_result()`**:** Assigns the result, i.e., the final point(s) to the instance.

Usage:

```
ResultAssignerArchive$assign_result(instance)
```

Arguments:

`instance` (bbotk::OptimInstanceBatchSingleCrit | bbotk::OptimInstanceBatchMultiCrit)
The bbotk::OptimInstance the final result should be assigned to.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

See Also

Other Result Assigner: ResultAssigner, mlr_result_assigners, mlr_result_assigners_surrogate

Examples

```
result_assigner = ras("archive")
```

---

mlr_result_assigners_surrogate

Result Assigner Based on a Surrogate Mean Prediction

Description

Result assigner that chooses the final point(s) based on a surrogate mean prediction of all evaluated points in the bbotk::Archive. This is especially useful in the case of noisy objective functions.

In the case of operating on an bbotk::OptimInstanceBatchMultiCrit the SurrogateLearnerCollection must use as many learners as there are objective functions.

Super class

mlr3mbo::ResultAssigner -> ResultAssignerSurrogate

Active bindings

surrogate (Surrogate | NULL)
: The surrogate.

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().

Methods

Public methods:

- ResultAssignerSurrogate$new()
- ResultAssignerSurrogate$assign_result()
- ResultAssignerSurrogate$clone()

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

Usage:

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

Arguments:

surrogate (Surrogate | NULL)
: The surrogate that is used to predict the mean of all evaluated points.

Method assign_result(): Assigns the result, i.e., the final point(s) to the instance. If $surrogate is NULL, default_surrogate(instance) is used and also assigned to $surrogate.

Usage:

```
ResultAssignerSurrogate$assign_result(instance)
```

Arguments:

`instance` (bbotk::OptimInstanceBatchSingleCrit | bbotk::OptimInstanceBatchMultiCrit)
The bbotk::OptimInstance the final result should be assigned to.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

See Also

Other Result Assigner: `ResultAssigner`, `mlr_result_assigners`, `mlr_result_assigners_archive`

Examples

```
result_assigner = ras("surrogate")
```

`mlr_tuners_mbo` *TunerBatch 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::TunerBatch` -> `mlr3tuning::TunerBatchFromOptimizerBatch` -> `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_assigner` (ResultAssigner | `NULL`)
The result assigner.

`param_classes` (`character()`)
Supported parameter classes that the optimizer can optimize. Determined based on the `surrogate` and the `acq_optimizer`. This corresponds to the values given by a paradox::ParamSet's `$class` field.

`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 `acq_function`, `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_assigner = 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_assigner` (ResultAssigner | `NULL`)
The result assigner.

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_assigner`

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 = rsmp("cv", folds = 3)
  measure = msr("classif.acc")

  instance = TuningInstanceBatchSingleCrit$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 = TuningInstanceBatchMultiCrit$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)
}
```

`ras` *Syntactic Sugar Result Assigner Construction*

Description

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

Usage

```
ras(.key, ...)
```

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.

Value

ResultAssigner

Examples

```
ras("archive")
```

`ResultAssigner` *Result Assigner Base Class*

Description

Abstract result assigner class.

A result assigner is responsible for assigning the final optimization result to the bbotk::OptimInstance. Normally, it is only used within an OptimizerMbo.

Active bindings

`label (character(1))`
Label for this object.

`man (character(1))`
String in the format `[pkg]::[topic]` pointing to a manual page for this object.

`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()`.

Methods

Public methods:

- `ResultAssigner$new()`
- `ResultAssigner$assign_result()`
- `ResultAssigner$format()`
- `ResultAssigner$print()`
- `ResultAssigner$clone()`

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

Usage:

```
ResultAssigner$new(label = NA_character_, man = NA_character_)
```

Arguments:

`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 `assign_result()`**:** Assigns the result, i.e., the final point(s) to the instance.

Usage:

```
ResultAssigner$assign_result(instance)
```

Arguments:

`instance` (bbotk::OptimInstanceBatchSingleCrit | bbotk::OptimInstanceBatchMultiCrit)
The bbotk::OptimInstance the final result should be assigned to.

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

Usage:

```
ResultAssigner$format()
```

Returns: (`character(1)`).

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

Usage:

```
ResultAssigner$print()
```

Returns: (`character()`).

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

See Also

Other Result Assigner: `mlr_result_assigners`, `mlr_result_assigners_archive`, `mlr_result_assigners_surrogate`

`srlrn` *Syntactic Sugar Surrogate Construction*

Description

This function allows to construct a SurrogateLearner or SurrogateLearnerCollection in the spirit of `mlr_sugar` from **mlr3**.

If the `archive` references more than one target variable or `cols_y` contains more than one target variable but only a single `learner` is specified, this learner is replicated as many times as needed to build the SurrogateLearnerCollection.

Usage

```
srlrn(learner, archive = NULL, cols_x = NULL, cols_y = NULL, ...)
```

Arguments

`learner`	(mlr3::LearnerRegr | List of mlr3::LearnerRegr) mlr3::LearnerRegr that is to be used within the SurrogateLearner or a list of mlr3::LearnerRegr that are to be used within the SurrogateLearnerCollection.
`archive`	(`NULL` | bbotk::Archive) bbotk::Archive of the bbotk::OptimInstance used. Can also be `NULL`.
`cols_x`	(`NULL` | `character()`) Column ids in the bbotk::Archive that should be used as features. Can also be `NULL` in which case this is automatically inferred based on the archive.

`cols_y` (`NULL` | `character()`)
Column id(s) in the bbotk::Archive that should be used as a target. If a list of mlr3::LearnerRegr is provided as the `learner` argument and `cols_y` is specified as well, as many column names as learners must be provided. Can also be `NULL` in which case this is automatically inferred based on the archive.

`...` (named `list()`)
Named arguments passed to the constructor, to be set as parameters in the paradox::ParamSet.

Value

SurrogateLearner | SurrogateLearnerCollection

Examples

```
library(mlr3)
srlrn(lrn("regr.featureless"), catch_errors = FALSE)
srlrn(list(lrn("regr.featureless"), lrn("regr.featureless")))
```

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

`learner` (learner)
Arbitrary learner 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.

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

`cols_y` (`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_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:

- `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(learner, archive, cols_x, cols_y, param_set)
```

Arguments:

`learner` (learner)
Arbitrary learner object depending on the subclass.

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

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

`cols_y` (`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 learner 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()
```

Returns: (`character(1)`).

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 acquisition function 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, cols_x = NULL, col_y = NULL)
```

Arguments:

`learner` (mlr3::LearnerRegr).

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

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

`col_y` (`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 = OptimInstanceBatchSingleCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))

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

  instance$eval_batch(xdt)

  learner = default_gp()

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

  surrogate$update()

  surrogate$learner$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 `cols_y`. 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 use 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 acquisition function 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,
  cols_x = NULL,
  cols_y = NULL
)
```

Arguments:

`learners` (list of mlr3::LearnerRegr).

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

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

`cols_y` (`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 `col_y`.

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

  instance$eval_batch(xdt)

  learner1 = default_gp()

  learner2 = default_rf()

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

  surrogate$update()

  surrogate$learner
```

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

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