Package ‘mlr3mbo’

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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

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 paramdox::ParamSet, or to be set as public field. See mlr3misc::dictionary_sugar_get() for more details.
AcqFunction

Value

AcqFunction

Examples

acqf("ei")

---

AcqFunction Acquisition Function Base Class

Description

Abstract acquisition function class. Based on the predictions of a Surrogate, the acquisition function encodes the preference to evaluate a new point.

Super class

bbotk::Objective -> AcqFunction

Active bindings

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

surrogate_max_to_min (-1 | 1)
  Multiplicative factor to correct for minimization or maximization of the acquisition function.

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

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

archive (bbotk::Archive)
  Points to the bbotk::Archive of the surrogate.

fun (function)
  Pointing to the private acquisition function to be implemented by subclasses.

surrogate (Surrogate)
  Surrogate.

requires_predict_type_se (logical(1))
  Whether the acquisition function requires the surrogate to have "se" as $predict_type.

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:

```r
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:

```r
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:
dee Whether to make a deep clone.

See Also

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

acqo

Syntactic Sugar Acquisition Function Optimizer Construction

Description

This function allows to construct an AcqOptimizer in the spirit of mlr_sugar from mlr3.

Usage

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

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.

... (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 infill optimization. Wraps an bbotk::Optimizer and bbotk::Terminator.

Parameters

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

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

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

skip_already_evaluated logical(1)
It can happen that the candidate resulting of the infill optimization was already evaluated in a previous iteration. Should this candidate proposal be ignored and the next best point be selected as a candidate? Default is TRUE.
catch_errors logical(1)
Should errors during the infill optimization be caught and propagated to the loop_function
which can then handle the failed infill optimization appropriately by, e.g., proposing a randomly sampled point for evaluation? Default is TRUE.

Public fields
- optimizer (bbotk::Optimizer).
- terminator (bbotk::Terminator).
- acq_function (AcqFunction).

Active bindings
- print_id (character)
  Id used when printing.
- param_set (paradox::ParamSet)
  Set of hyperparameters.

Methods

Public methods:
- AcqOptimizer$new()
- AcqOptimizer$format()
- AcqOptimizer$print()
- AcqOptimizer$optimize()
- AcqOptimizer$clone()

Method new(): Creates a new instance of this R6 class.
Usage:
AcqOptimizer$new(optimizer, terminator, acq_function = NULL)

Arguments:
optimizer (bbotk::Optimizer).
terminator (bbotk::Terminator).
acq_function (NULL | AcqFunction).

Method format(): Helper for print outputs.
Usage:
AcqOptimizer$format()

Method print(): Print method.
Usage:
AcqOptimizer$print()

Returns: (character()).

Method optimize(): Optimize the acquisition function.
Usage:
AcqOptimizer$optimize()

Returns: `data.table::data.table()` with 1 row per optimum and x as columns.

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

Usage:
AcqOptimizer$clone(deep = FALSE)

Arguments:
deep Whether to make a deep clone.

---

### default_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**

```r
default_acqfunction(instance)
```

**Arguments**

- `instance` (`bbotk::OptimInstance`).

**Value**

`AcqFunction`

**See Also**

Other `mbo_defaults`: `default_acqoptimizer()`, `default_loop_function()`, `default_result_assigner()`, `default_surrogate()`, `mbo_defaults`
**Default Acquisition Function Optimizer**

**Description**

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

**Usage**

```r
default_acqoptimizer(acq_function)
```

**Arguments**

- `acq_function` (*AcqFunction*).

**Value**

`AcqOptimizer`

**See Also**

Other `mbo_defaults`: `default_acqfunction()`, `default_loop_function()`, `default_result_assigner()`, `default_surrogate()`, `mbo_defaults`

---

**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**

```r
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_result_assigner(),
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_loop_function(),
default_surrogate(), mbo_defaults

default_surrogate

Default Surrogate

Description

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

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

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

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

• A ranger regression forest ""regr.ranger"" with 500 trees is created.

• The standard error of a prediction (if required by the infill criterion) is estimated via jackknife. This is the se.method = "jack" option of the ""regr.ranger"" learner (default).

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

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

If the instance is of class bbotk::OptimInstanceSingleCrit the learner is wrapped as a SurrogateLearner.

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

Usage

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

Arguments

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

learner (NULL | mlr3::Learner).

n_learner (NULL | integer(1)).

Value

Surrogate

References

See Also

Other mbo_defaults: default_acqfunction(), default_acqoptimizer(), default_loop_function(), default_result_assigner(), 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_ego, mlr_loop_functions_emo, mlr_loop_functions_mpcl, mlr_loop_functions_parego, mlr_loop_functions_smsego, mlr_loop_functions

---

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_loop_function(), default_result_assigner(), default_surrogate()
**mlr_acqfunctions**

---

**Dictionary of Acquisition Functions**

### Description

A simple `mlr3misc::Dictionary` storing objects of class `AcqFunction`. Each acquisition function has an associated help page, see `mlr_acqfunctions_[id]`. For a more convenient way to retrieve and construct an acquisition function, see `acqf()`.

### Format

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

### Methods

See `mlr3misc::Dictionary`.

### See Also

- Sugar function: `acqf()`
- Other Dictionary: `mlr_loop_functions`, `mlr_result_assigners`
- Other Acquisition Function: `AcqFunction`, `mlr_acqfunctions_aei`, `mlr_acqfunctions_cb`, `mlr_acqfunctions_ehvigh`, `mlr_acqfunctions_ehvi`, `mlr_acqfunctions_eips`, `mlr_acqfunctions_ei`, `mlr_acqfunctions_mean`, `mlr_acqfunctions_pi`, `mlr_acqfunctions_sd`, `mlr_acqfunctions_smsego`

### Examples

```r
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()`:

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

Arguments:
- `surrogate` (NULL | SurrogateLearner).
- `c` (numeric(1)).

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

Usage:
```r
AcqFunctionAEI$update()
```

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

Usage:
```r
AcqFunctionAEI$clone(deep = FALSE)
```

Arguments:
- `deep` Whether to make a deep clone.

References

See Also

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

Examples

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

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

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

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

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

surrogate = srlrn(learner, archive = instance$archive)
acq_function = acqf("aei", surrogate = surrogate)
acq_function$surrogate$update()
acq_function$update()
acq_function$eval_dt(data.table(x = c(-1, 0, 1)))
}
```
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


See Also

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

Examples

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

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

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

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

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

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

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

  acq_function$surrogate$update()
  acq_function$eval_dt(data.table(x = c(-1, 0, 1)))
}
```
**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():** Updates acquisition function and sets `ys_front`, `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


See Also

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

Examples

```r
if (requireNamespace("mlr3learners") & requireNamespace("DiceKriging") & requireNamespace("rgenoud")) {
  library(bbotk)
  library(paradox)
  library(mlr3learners)
  library(data.table)
  fun = function(xs) {
    list(y1 = xs$x^2, y2 = (xs$x - 2)^2)
  }
  domain = ps(x = p_dbl(lower = -10, upper = 10))
  codomain = ps(y1 = p_dbl(tags = "minimize"), y2 = p_dbl(tags = "minimize"))
  objective = ObjectiveRFun$new(fun = fun, domain = domain, codomain = codomain)
  instance = OptimInstanceMultiCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))
  instance$eval_batch(data.table(x = c(-6, -5, 3, 9)))
  learner = lrn("regr.km",
    covtype = "matern3_2",
    optim.method = "gen",
    nugget.stability = 10^-8,
    control = list(trace = FALSE))
  surrogate = srlrn(list(learner, learner$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)))
}
```
Acquisition Function Expected Hypervolume Improvement via Gauss-Hermite Quadrature

Description


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(): Updates acquisition function and sets ys_front, ref_point, hypervolume, 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


See Also

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

Examples

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

fun = function(xs) {
  list(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"))
optimizer = ObjectiveRFun$new(fun = fun, domain = domain, codomain = codomain)

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

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

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

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

#### Super classes

bbotk::Objective -> mlr3mbo::AcqFunction -> AcqFunctionEI
Public fields

y_best (numeric(1))

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

Methods

Public methods:

• AcqFunctionEI$new()
• AcqFunctionEI$update()
• AcqFunctionEI$clone()

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

Usage:
AcqFunctionEI$new(surrogate = NULL)

Arguments:
surrogate (NULL | SurrogateLearner).

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

Usage:
AcqFunctionEI$update()

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

Usage:
AcqFunctionEI$clone(deep = FALSE)

Arguments:
deep Whether to make a deep clone.

References


See Also

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

Examples

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

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

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

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

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

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

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

mlr_acqfunctions_eips  Acquisition Function Expected Improvement Per Second

Description

Expected Improvement per Second.

It is assumed that calculations are performed on an bbotk::OptimInstanceSingleCrit. Additionally to target values of the codomain that should be minimized or maximized, the bbotk::Objective of the bbotk::OptimInstanceSingleCrit should return time values. The column names of the target variable and time variable must be passed as 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()`: Updates acquisition function and sets `y_best`.

Usage:

```
AcqFunctionEIPS$update()
```

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

Usage:

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

Arguments:

- `deep` Whether to make a deep clone.

References


See Also

Other Acquisition Function: `AcqFunction`, `mlr_acqfunctions_aei`, `mlr_acqfunctions_cb`, `mlr_acqfunctions_ehvigh`, `mlr_acqfunctions_ehvl`, `mlr_acqfunctions_ei`, `mlr_acqfunctions_mean`, `mlr_acqfunctions_pi`, `mlr_acqfunctions_sd`, `mlr_acqfunctions_smsego`, `mlr_acqfunctions`
Examples

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

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

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

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

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

  surrogate = 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_mean

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

Super classes

bbotk::Objective -> mlr3mbo::AcqFunction -> AcqFunctionMean

Methods

Public methods:

• AcqFunctionMean$new()
• AcqFunctionMean$clone()

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

Usage:
AcqFunctionMean$new(surrogate = NULL)

Arguments:
surrogate (NULL | SurrogateLearner).

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

Usage:
AcqFunctionMean$clone(deep = FALSE)

Arguments:
deep Whether to make a deep clone.

See Also

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

Examples

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

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

Acquisition Function Probability of Improvement

Description

Probability of Improvement.

Dictionary

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

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

Super classes

bbotk::Objective -> mlr3mbo::AcqFunction -> AcqFunctionPI

Public fields

y_best (numeric(1))

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

Public methods:

• `AcqFunctionPI$new()`
• `AcqFunctionPI$update()`
• `AcqFunctionPI$clone()`

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

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

Arguments:

`surrogate` (NULL | SurrogateLearner).

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

Usage:
`AcqFunctionPI$update()`

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

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

Arguments:

`deep` Whether to make a deep clone.

References


See Also

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

Examples

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

  fun = function(xs) {
    list(y = xs$x ^ 2)
  }

  domain = ps(x = p_dbl(lower = -10, upper = 10))
}
codomain = ps(y = p_dbl(tags = "minimize"))
objective = ObjectiveRFun$new(fun = fun, domain = domain, codomain = codomain)

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

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

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

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

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

mldr_acqfunctions_sd  Acquisition Function Standard Deviation

Description
Posterior Standard Deviation.

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

mldr_acqfunctions$get("sd")
acqf("sd")

Super classes
bbotk::Objective -> mldr3mbo::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_aei, mlr_acqfunctions_cb, mlr_acqfunctions_ehvigh, mlr_acqfunctions_ehvi, mlr_acqfunctions_eips, mlr_acqfunctions_ei, mlr_acqfunctions_mean, mlr_acqfunctions_pi, mlr_acqfunctions_smsego, mlr_acqfunctions

Examples

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

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

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

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

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

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

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

---

**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 = \((1 - 2 * \text{dnorm}(\text{lambda}))^m\) 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()`: Updates acquisition function and sets `ys_front`, `ref_point`, `epsilon`.

Usage:
`AcqFunctionSmsEgo$update()`

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

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

Arguments:
- `deep` Whether to make a deep clone.

References


See Also

Other Acquisition Function: `AcqFunction`, `mlr_acqfunctions_aei`, `mlr_acqfunctions_cb`, `mlr_acqfunctions_ehvigh`, `mlr_acqfunctions_ehv1`, `mlr_acqfunctions_eips`, `mlr_acqfunctions_ei`, `mlr_acqfunctions_mean`, `mlr_acqfunctions_pi`, `mlr_acqfunctions_sd`, `mlr_acqfunctions`
Examples

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

  library(bbotk)
  library(paradox)
  library(mlr3learners)
  library(data.table)

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

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

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

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

  surrogate = 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)).

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)

---

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::OptimInstanceSingleCrit)
  The bbotk::OptimInstanceSingleCrit 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::OptimInstanceSingleCrit.

References


See Also

Other Loop Function: *loop_function, mlr_loop_functions_emo, mlr_loop_functions_mpcl, mlr_loop_functions_parego, mlr_loop_functions_smsego, mlr_loop_functions*
Examples

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

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

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

  instance = OptimInstanceSingleCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))
  surrogate = default_surrogate(instance)
  acq_function = acqf("ei")
  acq_optimizer = acqo(
    optimizer = opt("random_search", batch_size = 100),
    terminator = trm("evals", n_evals = 100))
  optimizer = opt("mbo",
    loop_function = bayesopt_ego,
    surrogate = surrogate,
    acq_function = acq_function,
    acq_optimizer = acq_optimizer)

  optimizer$optimize(instance)

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

  instance = OptimInstanceSingleCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))
  surrogate = default_surrogate(instance, n_learner = 2)
  surrogate$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::OptimInstanceMultiCrit)
    The bbotk::OptimInstanceMultiCrit 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::OptimInstanceMultiCrit.

See Also
Other Loop Function: loop_function, mlr_loop_functions_ego, mlr_loop_functions_mpcl, mlr_loop_functions_parego, mlr_loop_functions_smsego, mlr_loop_functions

Examples
if (requireNamespace("mlr3learners") & requireNamespace("DiceKriging") & requireNamespace("rgenoud")) {
  library(bbotk)
  library(paradox)
  library(mlr3learners)
  fun = function(xs) {
    list(y1 = xs$x^2, y2 = (xs$x - 2) ^ 2)
  }
  domain = ps(x = p_dbl(lower = -10, upper = 10))
  codomain = ps(y1 = p_dbl(tags = "minimize"), y2 = p_dbl(tags = "minimize"))
  objective = ObjectiveRFun$new(fun = fun, domain = domain, codomain = codomain)
  instance = OptimInstanceMultiCrit$new(
    objective = objective,
    terminator = trm("evals", n_evals = 5))
  surrogate = default_surrogate(instance)
acq_function = acqf("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)

---

**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**

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

**Arguments**

- `instance` (bbotk::OptimInstanceSingleCrit)
  The bbotk::OptimInstanceSingleCrit 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::OptimInstanceSingleCrit.
• To make use of parallel evaluations in the case of ‘q > 1, the objective function of the bbotk::OptimInstanceSingleCrit must be implemented accordingly.

References
See Also

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

Examples

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

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

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

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

  surrogate = default_surrogate(instance)

  acq_function = acqf("ei")

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

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

  optimizer$optimize(instance)
}
```
**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**

```r
bayesopt_parego(
  instance,  # bbotk::OptimInstanceMultiCrit
  surrogate, # SurrogateLearner
  acq_function,  # AcqFunction
  acq_optimizer,  # AcqOptimizer
  init_design_size = NULL,  # NULL | integer(1)
  q = 1L,  # integer(1)
  s = 100L,  # integer(1)
  rho = 0.05,  # numeric(1)
  random_interleave_iter = 0L
)
```

**Arguments**

- **instance** (bbotk::OptimInstanceMultiCrit)
  The `bbotk::OptimInstanceMultiCrit` 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, \( 4 \times d \) 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))
  \( \rho \) 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::OptimInstanceMultiCrit.
- The scalarizations of the objective function values are stored as the y_scal column in the bbotk::Archive of the bbotk::OptimInstanceMultiCrit.
- To make use of parallel evaluations in the case of ‘q > 1, the objective function of the bbotk::OptimInstanceMultiCrit must be implemented accordingly.

References


See Also

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

Examples

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

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

fun = function(xs) {

```r
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"))
optimum = ObjectiveRFun$new(fun = fun, domain = domain, codomain = codomain)

instance = OptimInstanceMultiCrit$new(
  objective = optimum,
  terminator = trm("evals", n_evals = 5))
surrogate = default_surrogate(instance, n_learner = 1)

acq_function = acq("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**

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

instance (bbotk::OptimInstanceMultiCrit)
The bbotk::OptimInstanceMultiCrit 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::OptimInstanceMultiCrit.
- Due to the iterative computation of the epsilon within the mlr_acqfunctions_smsego, requires
  the bbotk::Terminator of the bbotk::OptimInstanceMultiCrit to be a bbotk::TerminatorEvals.

References

  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
See Also

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

Examples

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

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

fun = function(xs) {
  list(y1 = xs$x^2, y2 = (xs$x - 2) ^ 2)
}

domain = ps(x = p_dbl(lower = -10, upper = 10))
codomain = ps(y1 = p_dbl(tags = "minimize"), y2 = p_dbl(tags = "minimize"))

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

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

surrogate = default_surrogate(instance)

acq_function = acqf("smsego")

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

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

optimizer$optimize(instance)
}
```
Description

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

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

Termination is handled via a bbotk::Terminator part of the bbotk::OptimInstance to be optimized.

Archive

The bbotk::Archive holds the following additional columns that are specific to MBO algorithms:

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

Super class

bbotk::Optimizer -> OptimizerMbo

Active bindings

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

surrogate (Surrogate | NULL)
  The surrogate.

acq_function (AcqFunction | NULL)
  The acquisition function.

acq_optimizer (AcqOptimizer | NULL)
  The acquisition function optimizer.

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

result_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. Subclasses of paradox::Param.
properties (character())
  Set of properties of the optimizer. Must be a subset of `bbotk_reflections$optimizer_properties`. MBO in principle is very flexible and by default we assume that the optimizer has all properties. When fully initialized, properties are determined based on the `loop_function` and `surrogate`.

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

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

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

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

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

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

surrogate = srlrn(learner)

acq_function = acqf("ei")

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

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

optimizer$optimize(instance)

# multi-objective ParEGO
fun = function(xs) {
  list(y1 = xs$x^2, y2 = (xs$x - 2)^2)
}

domain = ps(x = p_dbl(lower = -10, upper = 10))
codomain = ps(y1 = p_dbl(tags = "minimize"), y2 = p_dbl(tags = "minimize"))
optimizer = ObjectiveRFun$new(fun = fun, domain = domain, codomain = codomain)

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

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

optimizer$optimize(instance)

---

**mlr_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.
mlr_result_assigners_archive

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::OptimInstanceSingleCrit | bbotk::OptimInstanceMultiCrit)
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_surrogate, mlr_result_assigners

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::OptimInstanceMultiCrit 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::OptimInstanceSingleCrit | bbotk::OptimInstanceMultiCrit)
  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_archive`, `mlr_result_assigners`

Examples

`result_assigner = ras("surrogate")`
Description

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

Super classes

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

Active bindings

- loop_function (loop_function | NULL)
  Loop function determining the MBO flavor.
- surrogate (Surrogate | NULL)
  The surrogate.
- acq_function (AcqFunction | NULL)
  The acquisition function.
- acq_optimizer (AcqOptimizer | NULL)
  The acquisition function optimizer.
- args (named list())
  Further arguments passed to the loop_function. For example, random_interleave_iter.
- result_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. Subclasses of paradox::Param.
- properties (character())
  Set of properties of the optimizer. Must be a subset of bbotk_reflections$optimizer_properties. MBO in principle is very flexible and by default we assume that the optimizer has all properties. When fully initialized, properties are determined based on the loop_function and surrogate.
- packages (character())
  Set of required packages. A warning is signaled prior to optimization if at least one of the packages is not installed, but loaded (not attached) later on-demand via requireNamespace(). Required packages are determined based on the acq_function, surrogate and the acq_optimizer.

Methods

Public methods:

- TunerMbo$new()
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

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

  tnr("mbo")$optimize(instance)

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

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

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

---

**Syntactic Sugar Result Assigner Construction**

**Description**

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

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 `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 `bboot::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()`
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::OptimInstanceSingleCrit | bbotk::OptimInstanceMultiCrit)
  The bbotk::OptimInstance the final result should be assigned to.

Method format(): Helper for print outputs.

Usage:
ResultAssigner$format()

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_archive, mlr_result_assigners_surrogate, mlr_result_assigners
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**

```r
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.

**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$predict()`
- `Surrogate$formatter()`
- `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()`
**SurrogateLearner**

Method `print()`: Print method.

Usage:

```r
Surrogate$print()
```

Returns: (character()).

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

Usage:

```r
Surrogate$clone(deep = FALSE)
```

Arguments:

depth Whether to make a deep clone.

---

**Surrogate Learner**  
*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 used to assert the insample performance of the `mlr3::LearnerRegr`. Only relevant if `assert_insample_perf = TRUE`. Default is `mlr3::mlr_measures_regr.rsq`.

- `perf_threshold` numeric(1)
  
  Threshold the insample performance of the `mlr3::LearnerRegr` should be asserted against. Only relevant if `assert_insample_perf = TRUE`. Default is `0`.

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

**Super class**

`mlr3mbo::Surrogate` -> SurrogateLearner
Active bindings

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

Methods

**Public methods:**

- `SurrogateLearner$new()`
- `SurrogateLearner$predict()`
- `SurrogateLearner$clone()`

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

**Usage:**

```r
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:**

```r
SurrogateLearner$predict(xdt)
```

**Arguments:**
SurrogateLearner

xdt (\texttt{data.table::data.table()})

New data. One row per observation.

Returns: \texttt{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:
dee \textbf{p} Whether to make a deep clone.

Examples

\begin{verbatim}
if (requireNamespace("mlr3learners") &
    requireNamespace("DiceKriging") &
    requireNamespace("rgenoud")) {
    library(bbotk)
    library(paradox)
    library(mlr3learners)

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

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

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

    instance$eval_batch(xdt)

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

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

    surrogate$update()

    surrogate$learner$model
  }
\end{verbatim}
**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 used to assert the insample performance of the `mlr3::LearnerRegr`. Only relevant if `assert_insample_perf = TRUE`. Default is `mlr3::mlr_measures_regr.rsq` for each learner.

- `perf_threshold` List of numeric(1)
  Thresholds the insample performance of the `mlr3::LearnerRegr` should be asserted against. Only relevant if `assert_insample_perf = TRUE`. Default is 0 for each learner.

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

**Super class**

`mlr3mbo::Surrogate` $>$ SurrogateLearnerCollection

**Active bindings**

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

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

- `assert_insample_perf` (numeric())
  Asserts whether the current insample performance meets the performance threshold.

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

- `feature_types` (character())
  Stores the feature types the surrogate can handle, e.g. "logical", "numeric", or "factor". A complete list of candidate feature types, grouped by task type, is stored in `mlr_reflections$task_feature_types`.
properties (character())
Stores a set of properties/capabilities the surrogate has. A complete list of candidate properties, grouped by task type, is stored in mlr_reflections$learner_properties.
predict_type (character(1))
Retrieves the currently active predict type, e.g. "response".

Methods

Public methods:
• SurrogateLearnerCollection$new()
• SurrogateLearnerCollection$predict()
• SurrogateLearnerCollection$clone()

Method new(): Creates a new instance of this R6 class.
Usage:
SurrogateLearnerCollection$new(
  learners,
  archive = NULL,
  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:
deeipt whether to make a deep clone.
Examples

```r
if (requireNamespace("mlr3learners") &
    requireNamespace("DiceKriging") &
    requireNamespace("rgenoud") &
    requireNamespace("ranger")) {
  library(bbock)
  library(paradox)
  library(mlr3learners)

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

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

  instance$eval_batch(xdt)

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

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

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

  surrogate$learner

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