

Package ‘mlr3hyperband’

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Title Hyperband for 'mlr3'

Version 0.1.2

Description Implements hyperband method for hyperparameter tuning. Various termination criteria can be set and combined. The class 'AutoTuner' provides a convenient way to perform nested resampling in combination with 'mlr3'. The hyperband algorithm was proposed by Lisha Li, Kevin Jamieson, Giulia DeSalvo, Afshin Rostamizadeh and Ameet Talwalkar (2018) <arXiv:1603.06560>.

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URL <https://mlr3hyperband.mlr-org.com>,
<https://github.com/mlr-org/mlr3hyperband>

BugReports <https://github.com/mlr-org/mlr3hyperband/issues>

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mlr3hyperband-package *mlr3hyperband: Hyperband for 'mlr3'*

Description

Implements hyperband method for hyperparameter tuning. Various termination criteria can be set and combined. The class 'AutoTuner' provides a convenient way to perform nested resampling in combination with 'mlr3'. The hyperband algorithm was proposed by Lisha Li, Kevin Jamieson, Giulia DeSalvo, Afshin Rostamizadeh and Ameet Talwalkar (2018) <arXiv:1603.06560>.

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See Also

Useful links:

- <https://mlr3hyperband.ml-org.com>
- <https://github.com/mlr-org/mlr3hyperband>
- Report bugs at <https://github.com/mlr-org/mlr3hyperband/issues>

Description

TunerHyperband class that implements hyperband tuning. Hyperband is a budget oriented-procedure, weeding out suboptimal performing configurations early in a sequential training process, increasing tuning efficiency as a consequence.

For this, several brackets are constructed with an associated set of configurations for each bracket. Each bracket as several stages. Different brackets are initialized with different amounts of configurations and different budget sizes. To get an idea of how the bracket layout looks like for a given argument set, please have a look in the details.

To identify the budget for evaluating hyperband, the user has to specify explicitly which hyperparameter of the learner influences the budget by tagging a single hyperparameter in the `paradox::ParamSet` with "budget". An alternative approach using subsampling and pipelines is described below.

Naturally, hyperband terminates once all of its brackets are evaluated, so a `bbotk::Terminator` in the tuning instance acts as an upper bound and should be only set to a low value if one is unsure of how long hyperband will take to finish under the given settings.

Details

This sections explains the calculation of the constants for each bracket. A small overview will be given here, but for more details please check out the original paper (see references). To keep things uniform with the notation in the paper (and to save space in the formulas), R is used for the upper budget that last remaining configuration should reach. The formula to calculate the amount of brackets is $\text{floor}(\log(R, \text{eta})) + 1$. To calculate the starting budget in each bracket, use $R * \text{eta}^{-s}$, where s is the maximum bracket minus the current bracket index. For the starting configurations in each bracket it is $\text{ceiling}((B/R) * ((\text{eta}^s)/(s+1)))$, with $B = (\text{bracket amount}) * R$. To receive a table with the full brackets layout, load the following function and execute it for the desired R and eta .

```
hyperband_brackets = function(R, eta) {

  result = data.frame()
  smax = floor(log(R, eta))
  B = (smax + 1) * R

  # outer loop - iterate over brackets
  for (s in smax:0) {

    n = ceiling((B/R) * ((eta^s)/(s+1)))
    r = R * eta^(-s)

    # inner loop - iterate over bracket stages
    for (i in 0:s) {
```

```

    ni = floor(n * eta^(-i))
    ri = r * eta^i
    result = rbind(result, c(smax - s + 1, i + 1, ri, ni))
  }
}

names(result) = c("bracket", "bracket_stage", "budget", "n_configs")
return(result)
}

hyperband_brackets(R = 81L, eta = 3L)

```

Parameters

eta numeric(1)

Fraction parameter of the successive halving algorithm: With every step the configuration budget is increased by a factor of eta and only the best $1/\text{eta}$ configurations are used for the next stage. Non-integer values are supported, but eta is not allowed to be less or equal 1.

sampler [paradox::Sampler](#)

Object defining how the samples of the parameter space should be drawn during the initialization of each bracket. The default is uniform sampling.

Archive

The [mlr3tuning::ArchiveTuning](#) holds the following additional columns that are specific to the hyperband tuner:

- `bracket` (integer(1))
The console logs about the bracket index are actually not matching with the original hyperband algorithm, which counts down the brackets and stops after evaluating bracket 0. The true bracket indices are given in this column.
- `bracket_stage` (integer(1))
The bracket stage of each bracket. Hyperband starts counting at 0.
- `budget_scaled` (numeric(1))
The intermediate budget in each bracket stage calculated by hyperband. Because hyperband is originally only considered for budgets starting at 1, some rescaling is done to allow budgets starting at different values. For this, budgets are internally divided by the lower budget bound to get a lower budget of 1. Before the learner receives its budgets for evaluation, the budget is transformed back to match the original scale again.
- `budget_real` (numeric(1))
The real budget values the learner uses for evaluation after hyperband calculated its scaled budget.
- `n_configs` (integer(1))
The amount of evaluated configurations in each stage. These correspond to the r_i in the original paper.

Hyperband without learner budget

Thanks to **mlr3pipelines**, it is possible to use hyperband in combination with learners lacking a natural budget parameter. For example, any `mlr3::Learner` can be augmented with a `mlr3pipelines::PipeOp` operator such as `mlr3pipelines::PipeOpSubsample`. With the subsampling rate as budget parameter, the resulting `mlr3pipelines::GraphLearner` is fitted on small proportions of the `mlr3::Task` in the first brackets, and on the complete Task in last brackets. See examples for some code.

Custom sampler

Hyperband supports custom `paradox::Sampler` object for initial configurations in each bracket. A custom sampler may look like this (the full example is given in the examples section):

```
# - beta distribution with alpha = 2 and beta = 5
# - categorical distribution with custom probabilities
sampler = SamplerJointIndep$new(list(
  Sampler1DRfun$new(params[[2]], function(n) rbeta(n, 2, 5)),
  Sampler1DCateg$new(params[[3]], prob = c(0.2, 0.3, 0.5))
))
```

Runtime scaling w.r.t. the chosen budget

The calculation of each bracket currently assumes a linear runtime in the chosen budget parameter is always given. Hyperband is designed so each bracket requires approximately the same runtime as the sum of the budget over all configurations in each bracket is roughly the same. This will not hold true once the scaling in the budget parameter is not linear anymore, even though the sum of the budgets in each bracket remains the same. A basic example can be viewed by calling the function `hyperband_brackets` below with the arguments `R = 2` and `eta = 2`. If we run a learner with $O(\text{budget}^2)$ time complexity, the runtime of the last bracket will be 33% longer than the first bracket (time of bracket 1 = $2 * 1^2 + 2^2 = 6$; time of bracket 2 = $2 * 2^2 = 8$). Of course, this won't break anything, but it should be kept in mind when applying hyperband. A possible adaption would be to introduce a trafo, like it is shown in the examples.

Logging

When loading the `mlr3hyperband` package, two loggers based on the `lgr` package are made available. One is called `mlr3`, the other `bbotk`. All `mlr3` methods log into the `mlr3` logger. All optimization methods from the packages `bbotk`, `mlr3tuning` and `mlr3hyperband` log into the `bbotk` logger. To hide the `mlr3` logging messages run:

```
lgr::get_logger("mlr3")$set_threshold("warn")
```

Super class

```
mlr3tuning::Tuner -> TunerHyperband
```

Methods

Public methods:

- `TunerHyperband$new()`

- `TunerHyperband$clone()`

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

Usage:

```
TunerHyperband$new()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Source

Li L, Jamieson K, DeSalvo G, Rostamizadeh A, Talwalkar A (2018). “Hyperband: A Novel Bandit-Based Approach to Hyperparameter Optimization.” *Journal of Machine Learning Research*, **18**(185), 1-52. <https://jmlr.org/papers/v18/16-558.html>.

Examples

```
if(requireNamespace("xgboost")) {
  library(mlr3)
  library(mlr3learners)
  library(paradox)
  library(mlr3tuning)
  library(mlr3hyperband)

  # Define hyperparameter and budget parameter for tuning with hyperband
  ps = ParamSet$new(list(
    ParamInt$new("nrounds", lower = 1, upper = 4, tag = "budget"),
    ParamDbl$new("eta", lower = 0, upper = 1),
    ParamFct$new("booster", levels = c("gbtree", "gblinear", "dart"))
  ))

  # Define termination criterion
  # Hyperband terminates itself
  terminator = trm("none")

  # Create tuning instance
  inst = TuningInstanceSingleCrit$new(
    task = tsk("iris"),
    learner = lrn("classif.xgboost"),
    resampling = rsmpl("holdout"),
    measure = msr("classif.ce"),
    search_space = ps,
    terminator = terminator,
  )

  # Load tuner
  tuner = tnr("hyperband", eta = 2L)
```

```
# Trigger optimization
tuner$optimize(inst)

# Print all evaluations
as.data.table(inst$archive)
}
```

nds_selection

Best points w.r.t. non dominated sorting with hypervolume contrib.

Description

Select best subset of points by non dominated sorting with hypervolume contribution for tie breaking. Works on an arbitrary dimension of size two or higher. Returns a vector of indices of selected points.

Value

integer()

Parameters

points matrix()

Numeric matrix with each column corresponding to a point.

n_select integer(1)

Amount of points to select.

ref_point integer()

Reference point for hypervolume.

minimize logical()

Should the ranking be based on minimization? (Single bool for all dimensions, or vector of bools with each entry corresponding to each dimension).

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