

Package ‘mlr3resampling’

July 12, 2024

Type Package

Title Resampling Algorithms for 'mlr3' Framework

Version 2024.7.7

Description A supervised learning algorithm inputs a train set, and outputs a prediction function, which can be used on a test set. If each data point belongs to a group (such as geographic region, year, etc), then how do we know if it is possible to train on one group, and predict accurately on another group? Cross-validation can be used to determine the extent to which this is possible, by first assigning fold IDs from 1 to K to all data (possibly using stratification, usually by group and label). Then we loop over test sets (group/fold combinations), train sets (same group, other groups, all groups), and compute test/prediction accuracy for each combination. Comparing test/prediction accuracy between same and other, we can determine the extent to which it is possible (perfect if same/other have similar test accuracy for each group; other is usually somewhat less accurate than same; other can be just as bad as featureless baseline when the groups have different patterns). For more information, [<https://tdhock.github.io/blog/2023/R-gen-new-subsets/>](https://tdhock.github.io/blog/2023/R-gen-new-subsets/) describes the method in depth. How many train samples are required to get accurate predictions on a test set? Cross-validation can be used to answer this question, with variable size train sets.

License GPL-3

URL <https://github.com/tdhock/mlr3resampling>

BugReports <https://github.com/tdhock/mlr3resampling/issues>

Imports data.table, R6, checkmate, paradox, mlr3, mlr3misc

Suggests ggplot2, animint2, mlr3tuning, lgr, future, testthat, knitr, markdown, nc, rpart, directlabels

VignetteBuilder knitr

NeedsCompilation no

Author Toby Hocking [aut, cre] (<<https://orcid.org/0000-0002-3146-0865>>),
 Michel Lang [ctb] (<<https://orcid.org/0000-0001-9754-0393>>, Author of
 mlr3 when Resampling/ResamplingCV was copied/modified),
 Bernd Bischl [ctb] (<<https://orcid.org/0000-0001-6002-6980>>, Author of
 mlr3 when Resampling/ResamplingCV was copied/modified),
 Jakob Richter [ctb] (<<https://orcid.org/0000-0003-4481-5554>>, Author of
 mlr3 when Resampling/ResamplingCV was copied/modified),
 Patrick Schratz [ctb] (<<https://orcid.org/0000-0003-0748-6624>>, Author
 of mlr3 when Resampling/ResamplingCV was copied/modified),
 Giuseppe Casalicchio [ctb] (<<https://orcid.org/0000-0001-5324-5966>>,
 Author of mlr3 when Resampling/ResamplingCV was copied/modified),
 Stefan Coors [ctb] (<<https://orcid.org/0000-0002-7465-2146>>, Author of
 mlr3 when Resampling/ResamplingCV was copied/modified),
 Quay Au [ctb] (<<https://orcid.org/0000-0002-5252-8902>>, Author of mlr3
 when Resampling/ResamplingCV was copied/modified),
 Martin Binder [ctb],
 Florian Pfisterer [ctb] (<<https://orcid.org/0000-0001-8867-762X>>,
 Author of mlr3 when Resampling/ResamplingCV was copied/modified),
 Raphael Sonabend [ctb] (<<https://orcid.org/0000-0001-9225-4654>>, Author
 of mlr3 when Resampling/ResamplingCV was copied/modified),
 Lennart Schneider [ctb] (<<https://orcid.org/0000-0003-4152-5308>>,
 Author of mlr3 when Resampling/ResamplingCV was copied/modified),
 Marc Becker [ctb] (<<https://orcid.org/0000-0002-8115-0400>>, Author of
 mlr3 when Resampling/ResamplingCV was copied/modified),
 Sebastian Fischer [ctb] (<<https://orcid.org/0000-0002-9609-3197>>,
 Author of mlr3 when Resampling/ResamplingCV was copied/modified)

Maintainer Toby Hocking <toby.hocking@r-project.org>

Repository CRAN

Date/Publication 2024-07-12 15:50:02 UTC

Contents

AZtrees	2
ResamplingSameOtherCV	4
ResamplingSameOtherSizesCV	6
ResamplingVariableSizeTrainCV	9
score	11

Index 13

AZtrees

Arizona Trees

Description

Classification data set with polygons (groups which should not be split in CV) and subsets (region3 or region4).

Usage

```
data("AZtrees")
```

Format

A data frame with 5956 observations on the following 25 variables.

region3 a character vector

region4 a character vector

polygon a numeric vector

y a character vector

ycoord latitude

xcoord longitude

SAMPLE_1 a numeric vector

SAMPLE_2 a numeric vector

SAMPLE_3 a numeric vector

SAMPLE_4 a numeric vector

SAMPLE_5 a numeric vector

SAMPLE_6 a numeric vector

SAMPLE_7 a numeric vector

SAMPLE_8 a numeric vector

SAMPLE_9 a numeric vector

SAMPLE_10 a numeric vector

SAMPLE_11 a numeric vector

SAMPLE_12 a numeric vector

SAMPLE_13 a numeric vector

SAMPLE_14 a numeric vector

SAMPLE_15 a numeric vector

SAMPLE_16 a numeric vector

SAMPLE_17 a numeric vector

SAMPLE_18 a numeric vector

SAMPLE_19 a numeric vector

SAMPLE_20 a numeric vector

SAMPLE_21 a numeric vector

Source

Paul Nelson Arellano, paul.arellano@nau.edu

Examples

```
data(AZtrees)
task.obj <- mlr3::TaskClassif$new("AZtrees3", AZtrees, target="y")
task.obj$col_roles$feature <- grep("SAMPLE", names(AZtrees), value=TRUE)
task.obj$col_roles$group <- "polygon"
task.obj$col_roles$subset <- "region3"
str(task.obj)
same_other_sizes_cv <- mlr3resampling::ResamplingSameOtherSizesCV$new()
same_other_sizes_cv$instantiate(task.obj)
same_other_sizes_cv$instance$iteration.dt
```

ResamplingSameOtherCV *Resampling for comparing training on same or other groups*

Description

[ResamplingSameOtherCV](#) defines how a task is partitioned for resampling, for example in [resample\(\)](#) or [benchmark\(\)](#).

Resampling objects can be instantiated on a [Task](#), which should define at least one group variable.

After instantiation, sets can be accessed via `$train_set(i)` and `$test_set(i)`, respectively.

Details

A supervised learning algorithm inputs a train set, and outputs a prediction function, which can be used on a test set. If each data point belongs to a group (such as geographic region, year, etc), then how do we know if it is possible to train on one group, and predict accurately on another group? Cross-validation can be used to determine the extent to which this is possible, by first assigning fold IDs from 1 to K to all data (possibly using stratification, usually by group and label). Then we loop over test sets (group/fold combinations), train sets (same group, other groups, all groups), and compute test/prediction accuracy for each combination. Comparing test/prediction accuracy between same and other, we can determine the extent to which it is possible (perfect if same/other have similar test accuracy for each group; other is usually somewhat less accurate than same; other can be just as bad as featureless baseline when the groups have different patterns).

Stratification

[ResamplingSameOtherCV](#) supports stratified sampling. The stratification variables are assumed to be discrete, and must be stored in the [Task](#) with column role "stratum". In case of multiple stratification variables, each combination of the values of the stratification variables forms a stratum.

Grouping

[ResamplingSameOtherCV](#) supports grouping of observations. The grouping variable is assumed to be discrete, and must be stored in the [Task](#) with column role "group".

The number of cross-validation folds K should be defined as the `fold` parameter.

In each group, there will be about an equal number of observations assigned to each of the K folds. The assignments are stored in `$instance$id.dt`. The train/test splits are defined by all possible combinations of test group, test fold, and train groups (same/other/all). The splits are stored in `$instance$iteration.dt`.

Methods

Public methods:

- [Resampling\\$new\(\)](#)
- [Resampling\\$train_set\(\)](#)
- [Resampling\\$test_set\(\)](#)

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

Usage:

```
Resampling$new(
  id,
  param_set = ps(),
  duplicated_ids = FALSE,
  label = NA_character_,
  man = NA_character_
)
```

Arguments:

`id` (`character(1)`)
Identifier for the new instance.

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

`duplicated_ids` (`logical(1)`)
Set to TRUE if this resampling strategy may have duplicated row ids in a single training set or test set.

`label` (`character(1)`)
Label for the new instance.

`man` (`character(1)`)
String in the format `[pkg]::[topic]` pointing to a manual page for this object. The referenced help package can be opened via method `$help()`.

Method `train_set()`: Returns the row ids of the i-th training set.

Usage:

```
Resampling$train_set(i)
```

Arguments:

`i` (`integer(1)`)
Iteration.

Returns: (`integer()`) of row ids.

Method `test_set()`: Returns the row ids of the i-th test set.

Usage:

```
Resampling$test_set(i)
```

Arguments:

```
i (integer(1))
  Iteration.
```

Returns: (integer()) of row ids.

See Also

- Blog post <https://tdhock.github.io/blog/2023/R-gen-new-subsets/>
- Package **mlr3** for standard [Resampling](#), which does not support comparing train on same or other groups.
- [score](#) and Simulations vignette for more detailed examples.

Examples

```
same_other <- mlr3resampling::ResamplingSameOtherCV$new()
same_other$param_set$values$fold <- 5
```

ResamplingSameOtherSizesCV

Resampling for comparing train subsets and sizes

Description

[ResamplingSameOtherSizesCV](#) defines how a task is partitioned for resampling, for example in [resample\(\)](#) or [benchmark\(\)](#).

Resampling objects can be instantiated on a [Task](#), which should define at least one group variable.

After instantiation, sets can be accessed via `$train_set(i)` and `$test_set(i)`, respectively.

Details

A supervised learning algorithm inputs a train set, and outputs a prediction function, which can be used on a test set. If each data point belongs to a group (such as geographic region, year, etc), then how do we know if it is possible to train on one group, and predict accurately on another group? Cross-validation can be used to determine the extent to which this is possible, by first assigning fold IDs from 1 to K to all data (possibly using stratification, usually by group and label). Then we loop over test sets (group/fold combinations), train sets (same group, other groups, all groups), and compute test/prediction accuracy for each combination. Comparing test/prediction accuracy between same and other, we can determine the extent to which it is possible (perfect if same/other have similar test accuracy for each group; other is usually somewhat less accurate than same; other can be just as bad as featureless baseline when the groups have different patterns).

This class has more parameters/potential applications than [ResamplingSameOtherCV](#) and [ResamplingVariableSizeTrainC](#) which are older and should only be preferred for visualization purposes.

Stratification

[ResamplingSameOtherSizesCV](#) supports stratified sampling. The stratification variables are assumed to be discrete, and must be stored in the [Task](#) with column role "stratum". In case of multiple stratification variables, each combination of the values of the stratification variables forms a stratum.

Grouping

[ResamplingSameOtherSizesCV](#) supports grouping of observations. The grouping variable is assumed to be discrete, and must be stored in the [Task](#) with column role "group".

Subsets

[ResamplingSameOtherSizesCV](#) supports training on different subsets of observations. The subset variable is assumed to be discrete, and must be stored in the [Task](#) with column role "subset".

Parameters

The number of cross-validation folds K should be defined as the `fold` parameter, default 3.

The number of random seeds for down-sampling should be defined as the `seeds` parameter, default 1.

The ratio for down-sampling should be defined as the `ratio` parameter, default 0.5. The min size of same and other sets is repeatedly multiplied by this ratio, to obtain smaller sample sizes.

The number of down-sampling sizes/multiplications should be defined as the `sizes` parameter, which can also take two special values: default -1 means no down-sampling at all, and 0 means only down-sampling to the sizes of the same/other sets.

The `ignore_subset` parameter should be either TRUE or FALSE (default), whether to ignore the subset role. TRUE only creates splits for same subset (even if task defines subset role), and is useful for subtrain/validation splits (hyper-parameter learning). Note that this feature will work on a task with `stratum` and `group` roles (unlike [ResamplingCV](#)).

In each subset, there will be about an equal number of observations assigned to each of the K folds. The train/test splits are defined by all possible combinations of test subset, test fold, train subsets (same/other/all), down-sampling sizes, and random seeds. The splits are stored in `$instance$iteration.dt`.

Methods

Public methods:

- [Resampling\\$new\(\)](#)
- [Resampling\\$train_set\(\)](#)
- [Resampling\\$test_set\(\)](#)

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

Usage:

```
Resampling$new(
  id,
  param_set = ps(),
```

```

    duplicated_ids = FALSE,
    label = NA_character_,
    man = NA_character_
  )

```

Arguments:

```

id (character(1))
  Identifier for the new instance.
param_set (paradox::ParamSet)
  Set of hyperparameters.
duplicated_ids (logical(1))
  Set to TRUE if this resampling strategy may have duplicated row ids in a single training set
  or test set.
label (character(1))
  Label for the new instance.
man (character(1))
  String in the format [pkg]::[topic] pointing to a manual page for this object. The refer-
  enced help package can be opened via method $help().

```

Method `train_set()`: Returns the row ids of the *i*-th training set.

Usage:

```
Resampling$train_set(i)
```

Arguments:

```

i (integer(1))
  Iteration.

```

Returns: (integer()) of row ids.

Method `test_set()`: Returns the row ids of the *i*-th test set.

Usage:

```
Resampling$test_set(i)
```

Arguments:

```

i (integer(1))
  Iteration.

```

Returns: (integer()) of row ids.

See Also

- Blog post <https://tdhock.github.io/blog/2023/R-gen-new-subsets/>
- Package **mlr3** for standard [Resampling](#), which does not support comparing train on same or other groups.
- [score](#) and Simulations vignette for more detailed examples.

Examples

```

same_other_sizes <- mlr3resampling::ResamplingSameOtherSizesCV$new()
same_other_sizes$param_set$values$fold <- 5

```

ResamplingVariableSizeTrainCV

Resampling for comparing training on same or other groups

Description

[ResamplingVariableSizeTrainCV](#) defines how a task is partitioned for resampling, for example in `resample()` or `benchmark()`.

Resampling objects can be instantiated on a [Task](#).

After instantiation, sets can be accessed via `$train_set(i)` and `$test_set(i)`, respectively.

Details

A supervised learning algorithm inputs a train set, and outputs a prediction function, which can be used on a test set. How many train samples are required to get accurate predictions on a test set? Cross-validation can be used to answer this question, with variable size train sets.

Stratification

[ResamplingVariableSizeTrainCV](#) supports stratified sampling. The stratification variables are assumed to be discrete, and must be stored in the [Task](#) with column role "stratum". In case of multiple stratification variables, each combination of the values of the stratification variables forms a stratum.

Grouping

[ResamplingVariableSizeTrainCV](#) does not support grouping of observations.

Hyper-parameters

The number of cross-validation folds should be defined as the `fold` parameter.

For each fold ID, the corresponding observations are considered the test set, and a variable number of other observations are considered the train set.

The `random_seeds` parameter controls the number of random orderings of the train set that are considered.

For each random order of the train set, the `min_train_data` parameter controls the size of the smallest stratum in the smallest train set considered.

To determine the other train set sizes, we use an equally spaced grid on the log scale, from `min_train_data` to the largest train set size (all data not in test set). The number of train set sizes in this grid is determined by the `train_sizes` parameter.

Methods**Public methods:**

- [Resampling\\$new\(\)](#)
- [Resampling\\$train_set\(\)](#)
- [Resampling\\$test_set\(\)](#)

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

Usage:

```
Resampling$new(
  id,
  param_set = ps(),
  duplicated_ids = FALSE,
  label = NA_character_,
  man = NA_character_
)
```

Arguments:

`id` (character(1))
Identifier for the new instance.

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

`duplicated_ids` (logical(1))
Set to TRUE if this resampling strategy may have duplicated row ids in a single training set or test set.

`label` (character(1))
Label for the new instance.

`man` (character(1))
String in the format `[pkg]::[topic]` pointing to a manual page for this object. The referenced help package can be opened via method `$help()`.

Method `train_set()`: Returns the row ids of the i-th training set.

Usage:

```
Resampling$train_set(i)
```

Arguments:

`i` (integer(1))
Iteration.

Returns: (integer()) of row ids.

Method `test_set()`: Returns the row ids of the i-th test set.

Usage:

```
Resampling$test_set(i)
```

Arguments:

`i` (integer(1))
Iteration.

Returns: (integer()) of row ids.

Examples

```
(var_sizes <- mlr3resampling::ResamplingVariableSizeTrainCV$new())
```

score	<i>Score benchmark results</i>
-------	--------------------------------

Description

Computes a data table of scores.

Usage

```
score(bench.result, ...)
```

Arguments

`bench.result` Output of `benchmark()`.
`...` Additional arguments to pass to `bench.result$score`, for example measures.

Value

data table with scores.

Author(s)

Toby Dylan Hocking

Examples

```
N <- 100
library(data.table)
set.seed(1)
reg.dt <- data.table(
  x=runif(N, -2, 2),
  person=rep(1:2, each=0.5*N))
reg.pattern.list <- list(
  easy=function(x, person)x^2,
  impossible=function(x, person)(x^2+person*3)*(-1)^person)
reg.task.list <- list()
for(pattern in names(reg.pattern.list)){
  f <- reg.pattern.list[[pattern]]
  yname <- paste0("y_",pattern)
  reg.dt[, (yname) := f(x,person)+rnorm(N, sd=0.5)][]
  task.dt <- reg.dt[, c("x", "person", yname), with=FALSE]
  task.obj <- mlr3::TaskRegr$new(
    pattern, task.dt, target=yname)
  task.obj$col_roles$stratum <- "person"
  task.obj$col_roles$subset <- "person"
  reg.task.list[[pattern]] <- task.obj
```

```
}
same_other <- mlr3resampling::ResamplingSameOtherSizesCV$new()
reg.learner.list <- list(
  mlr3::LearnerRegrFeatureless$new()
)
if(requireNamespace("rpart")){
  reg.learner.list$rpart <- mlr3::LearnerRegrRpart$new()
}
(bench.grid <- mlr3::benchmark_grid(
  reg.task.list,
  reg.learner.list,
  same_other))
bench.result <- mlr3::benchmark(bench.grid)
bench.score <- mlr3resampling::score(bench.result)
if(require(animint2)){
  ggplot()+
    geom_point(aes(
      regr.mse, train.subsets, color=algorithm),
      shape=1,
      data=bench.score)+
    facet_grid(
      test.subset ~ task_id,
      labeller=label_both,
      scales="free")+
    scale_x_log10()
}
```

Index

* **Resampling**

ResamplingSameOtherCV, [4](#)

ResamplingSameOtherSizesCV, [6](#)

ResamplingVariableSizeTrainCV, [9](#)

* **datasets**

AZtrees, [2](#)

AZtrees, [2](#)

benchmark(), [4](#), [6](#), [9](#), [11](#)

paradox::ParamSet, [5](#), [8](#), [10](#)

R6, [5](#), [7](#), [10](#)

resample(), [4](#), [6](#), [9](#)

Resampling, [6](#), [8](#)

ResamplingSameOtherCV, [4](#), [4](#), [6](#)

ResamplingSameOtherSizesCV, [6](#), [6](#), [7](#)

ResamplingVariableSizeTrainCV, [6](#), [9](#), [9](#)

score, [6](#), [8](#), [11](#)

Task, [4](#), [6](#), [7](#), [9](#)