

Package ‘mlr3fselect’

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Title Feature Selection for 'mlr3'

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Description Implements methods for feature selection with 'mlr3', e.g. random search and sequential selection. Various termination criteria can be set and combined. The class 'AutoFSelector' provides a convenient way to perform nested resampling in combination with 'mlr3'.

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'extract_inner_fselect_archives.R'
'extract_inner_fselect_results.R' 'fselect.R'
'fselect_nested.R' 'FSelector.R' 'FSelectorFromOptimizer.R'
'FSelectorExhaustiveSearch.R' 'FSelectorRFE.R'
'FSelectorRandomSearch.R' 'FSelectorSequential.R'
'FSelectorShadowVariableSearch.R' 'FSelectorDesignPoints.R'
'FSelectorGeneticSearch.R' 'FSelectInstanceMultiCrit.R'
'FSelectInstanceSingleCrit.R' 'reexports.R' 'sugar.R'
'bibentries.R' 'zzz.R'

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mlr3fselect-package *mlr3fselect: Feature Selection for 'mlr3'*

Description

Implements methods for feature selection with 'mlr3', e.g. random search and sequential selection. Various termination criteria can be set and combined. The class 'AutoFSelector' provides a convenient way to perform nested resampling in combination with 'mlr3'.

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See Also

Useful links:

- <https://mlr3fselect.mlr-org.com>
- <https://github.com/mlr-org/mlr3fselect>
- Report bugs at <https://github.com/mlr-org/mlr3fselect/issues>

ArchiveFSelect

Logging Object for Evaluated Feature Sets

Description

Container around a `data.table::data.table()` which stores all evaluated feature sets and performance scores.

Data structure

The table (`$data`) has the following columns:

- One column for each feature of the task (`$search_space`).
- One column for each performance measure (`$codomain`).
- `runtime_learners` (`numeric(1)`)
Sum of training and predict times logged in learners per `mlr3::ResampleResult` / evaluation. This does not include potential overhead time.
- `timestamp` (`POSIXct`)
Time stamp when the evaluation was logged into the archive.
- `batch_nr` (`integer(1)`)
Feature sets are evaluated in batches. Each batch has a unique batch number.
- `uhash` (`character(1)`)
Connects each feature set to the resampling experiment stored in the `mlr3::BenchmarkResult`.

Each row corresponds to a single evaluation of a feature set.

The archive stores additionally a `mlr3::BenchmarkResult` (`$benchmark_result`) that records the resampling experiments. Each experiment corresponds to a single evaluation of a feature set. The table (`$data`) and the benchmark result (`$benchmark_result`) are linked by the `uhash` column. If the results are viewed with `as.data.table()`, both are joined automatically.

Analysis

For analyzing the feature selection results, it is recommended to pass the archive to `as.data.table()`. The returned data table is joined with the benchmark result which adds the `mlr3::ResampleResult` for each feature set.

The archive provides various getters (e.g. `$learners()`) to ease the access. All getters extract by position (`i`) or unique hash (`uhash`). For a complete list of all getters see the methods section.

The benchmark result (`$benchmark_result`) allows to score the feature sets again on a different measure. Alternatively, measures can be supplied to `as.data.table()`.

S3 Methods

- `as.data.table.ArchiveFSelect(x, unnest = NULL, exclude_columns = "uhash", measures = NULL)`

Returns a tabular view of all evaluated feature sets.

`ArchiveFSelect -> data.table::data.table()`

- `x` (`ArchiveFSelect`)
- `unnest` (`character()`)
Transforms list columns to separate columns. Set to `NULL` if no column should be unnested.
- `exclude_columns` (`character()`)
Exclude columns from table. Set to `NULL` if no column should be excluded.
- `measures` (list of `mlr3::Measure`)
Score feature sets on additional measures.

Super class

`bbotk::Archive -> ArchiveFSelect`

Public fields

`benchmark_result` (`mlr3::BenchmarkResult`)
Stores benchmark result.

Methods

Public methods:

- `ArchiveFSelect$learner()`
- `ArchiveFSelect$learners()`
- `ArchiveFSelect$predictions()`
- `ArchiveFSelect$resample_result()`
- `ArchiveFSelect$print()`
- `ArchiveFSelect$clone()`

Method `learner()`: Retrieve `mlr3::Learner` of the `i`-th evaluation, by position or by unique hash `uhash`. `i` and `uhash` are mutually exclusive. Learner does not contain a model. Use `$learners()` to get learners with models.

Usage:

```
ArchiveFSelect$learner(i = NULL, uhash = NULL)
```

Arguments:

i (integer(1))

The iteration value to filter for.

uhash (logical(1))

The uhash value to filter for.

Method `learners()`: Retrieve list of trained `mlr3::Learner` objects of the *i*-th evaluation, by position or by unique hash *uhash*. *i* and *uhash* are mutually exclusive.

Usage:

```
ArchiveFSelect$learners(i = NULL, uhash = NULL)
```

Arguments:

i (integer(1))

The iteration value to filter for.

uhash (logical(1))

The uhash value to filter for.

Method `predictions()`: Retrieve list of `mlr3::Prediction` objects of the *i*-th evaluation, by position or by unique hash *uhash*. *i* and *uhash* are mutually exclusive.

Usage:

```
ArchiveFSelect$predictions(i = NULL, uhash = NULL)
```

Arguments:

i (integer(1))

The iteration value to filter for.

uhash (logical(1))

The uhash value to filter for.

Method `resample_result()`: Retrieve `mlr3::ResampleResult` of the *i*-th evaluation, by position or by unique hash *uhash*. *i* and *uhash* are mutually exclusive.

Usage:

```
ArchiveFSelect$resample_result(i = NULL, uhash = NULL)
```

Arguments:

i (integer(1))

The iteration value to filter for.

uhash (logical(1))

The uhash value to filter for.

Method `print()`: Printer.

Usage:

```
ArchiveFSelect$print()
```

Arguments:

... (ignored).

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

AutoFSelector

AutoFSelector

Description

The `AutoFSelector` is a `mlr3::Learner` which wraps another `mlr3::Learner` and performs the following steps during `$train()`:

1. The wrapped (inner) learner is trained on the feature subsets via resampling. The feature selection can be specified by providing a `FSelector`, a `bbotk::Terminator`, a `mlr3::Resampling` and a `mlr3::Measure`.
2. A final model is fit on the complete training data with the best found feature subset.

During `$predict()` the `AutoFSelector` just calls the `predict` method of the wrapped (inner) learner.

Note that this approach allows to perform nested resampling by passing an `AutoFSelector` object to `mlr3::resample()` or `mlr3::benchmark()`. To access the inner resampling results, set `store_fselect_instance = TRUE` and execute `mlr3::resample()` or `mlr3::benchmark()` with `store_models = TRUE`.

Super class

```
mlr3::Learner -> AutoFSelector
```

Public fields

`instance_args` (`list()`)

All arguments from construction to create the `FSelectInstanceSingleCrit`.

`fselector` (`FSelector`)

Stores the feature selection algorithm.

Active bindings

`archive` (`[ArchiveFSelect]`)

Returns `FSelectInstanceSingleCrit` archive.

`learner` (`mlr3::Learner`)

Trained learner.

`fselect_instance` (`FSelectInstanceSingleCrit`)

Internally created feature selection instance with all intermediate results.

`fselect_result` (`data.table::data.table`)

Short-cut to `$result` from `FSelectInstanceSingleCrit`.

`hash` (`character(1)`)

Hash (unique identifier) for this object.

Methods

Public methods:

- [AutoFSelector\\$new\(\)](#)
- [AutoFSelector\\$base_learner\(\)](#)
- [AutoFSelector\\$clone\(\)](#)

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

Usage:

```
AutoFSelector$new(
  learner,
  resampling,
  measure,
  terminator,
  fselector,
  store_fselect_instance = TRUE,
  store_benchmark_result = TRUE,
  store_models = FALSE,
  check_values = FALSE
)
```

Arguments:

`learner` ([mlr3::Learner](#))

Learner to optimize the feature subset for, see [FSelectInstanceSingleCrit](#).

`resampling` ([mlr3::Resampling](#))

Resampling strategy during feature selection, see [FSelectInstanceSingleCrit](#). This [mlr3::Resampling](#) is meant to be the **inner** resampling, operating on the training set of an arbitrary outer resampling. For this reason it is not feasible to pass an instantiated [mlr3::Resampling](#) here.

`measure` ([mlr3::Measure](#))

Performance measure to optimize.

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

When to stop feature selection, see [FSelectInstanceSingleCrit](#).

`fselector` ([FSelector](#))

Feature selection algorithm to run.

`store_fselect_instance` (`logical(1)`)

If TRUE (default), stores the internally created [FSelectInstanceSingleCrit](#) with all intermediate results in slot `$fselect_instance`.

`store_benchmark_result` (`logical(1)`)

Store benchmark result in archive?

`store_models` (`logical(1)`). Store models in benchmark result?

`check_values` (`logical(1)`)

Check the parameters before the evaluation and the results for validity?

Method `base_learner()`: Extracts the base learner from nested learner objects like `GraphLearner` in [mlr3pipelines](#). If `recursive = 0`, the (tuned) learner is returned.

Usage:

```
AutoFSelector$base_learner(recursive = Inf)
```

Arguments:

recursive (integer(1))
 Depth of recursion for multiple nested objects.

Returns: [Learner](#).

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

Usage:

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

Arguments:

deep Whether to make a deep clone.

Examples

```
library(mlr3)

task = tsk("iris")
learner = lrn("classif.rpart")
resampling = rsmpl("holdout")
measure = msr("classif.ce")

terminator = trm("evals", n_evals = 3)
fselector = fs("exhaustive_search")
afs = AutoFSelector$new(learner, resampling, measure, terminator, fselector,
  store_fselect_instance = TRUE)

afs$train(task)
afs$model
afs$learner
```

 auto_fselector

Syntactic Sugar for Automatic Feature Selection

Description

Function to create an [AutoFSelector](#) object.

Usage

```
auto_fselector(
  method,
  learner,
  resampling,
  measure,
  term_evals = NULL,
  term_time = NULL,
  ...
)
```


Arguments

method	(character(1)) Key to retrieve fselector from mlr_fselectors dictionary.
learner	(mlr3::Learner).
resampling	(mlr3::Resampling) Uninstantiated resamplings are instantiated during construction so that all configurations are evaluated on the same data splits.
measure	(mlr3::Measure) Measure to optimize.
term_evals	(integer(1)) Number of allowed evaluations.
term_time	(integer(1)) Maximum allowed time in seconds.
...	(named list()) Named arguments to be set as parameters of the fselector.

Value[AutoFSelector](#)**Examples**

```
at = auto_fselector(
  method = "random_search",
  learner = lrn("classif.rpart"),
  resampling = rsmpl("holdout"),
  measure = msr("classif.ce"),
  term_evals = 4)

at$train(tsk("pima"))
```

 extract_inner_fselect_archives

Extract Inner Feature Selection Archives

Description

Extract inner feature selection archives of nested resampling. Implemented for [mlr3::ResampleResult](#) and [mlr3::BenchmarkResult](#). The function iterates over the [AutoFSelector](#) objects and binds the archives to a [data.table::data.table\(\)](#). [AutoFSelector](#) must be initialized with `store_fselect_instance = TRUE` and `resample()` or `benchmark()` must be called with `store_models = TRUE`.

Usage

```
extract_inner_fselect_archives(x, unnest = NULL, exclude_columns = "uhash")
```

Arguments

x	(mlr3::ResampleResult mlr3::BenchmarkResult).
unnest	(character()) Transforms list columns to separate columns. Set to NULL if no column should be unnested.
exclude_columns	(character()) Exclude columns from result table. Set to NULL if no column should be excluded.

Value

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

Data structure

The returned data table has the following columns:

- `experiment` ([integer\(1\)](#))
Index, giving the according row number in the original benchmark grid.
- `iteration` ([integer\(1\)](#))
Iteration of the outer resampling.
- One column for each feature of the task.
- One column for each performance measure.
- `runtime_learners` ([numeric\(1\)](#))
Sum of training and predict times logged in learners per [mlr3::ResampleResult](#) / evaluation. This does not include potential overhead time.
- `timestamp` ([POSIXct](#))
Time stamp when the evaluation was logged into the archive.
- `batch_nr` ([integer\(1\)](#))
Feature sets are evaluated in batches. Each batch has a unique batch number.
- `resample_result` ([mlr3::ResampleResult](#))
Resample result of the inner resampling.
- `task_id` ([character\(1\)](#)).
- `learner_id` ([character\(1\)](#)).
- `resampling_id` ([character\(1\)](#)).

Examples

```
at = auto_fselector(
  method = "random_search",
  learner = lrn("classif.rpart"),
  resampling = rsm("holdout"),
  measure = msr("classif.ce"),
  term_evals = 4)

resampling_outer = rsm("cv", folds = 2)
```

```
rr = resample(tsk("iris"), at, resampling_outer, store_models = TRUE)

extract_inner_fselect_archives(rr)
```

extract_inner_fselect_results

Extract Inner Feature Selection Results

Description

Extract inner feature selection results of nested resampling. Implemented for [mlr3::ResampleResult](#) and [mlr3::BenchmarkResult](#). The function iterates over the [AutoFSelector](#) objects and binds the feature selection results to a [data.table::data.table\(\)](#). [AutoFSelector](#) must be initialized with `store_fselect_instance = TRUE` and `resample()` or `benchmark()` must be called with `store_models = TRUE`.

Usage

```
extract_inner_fselect_results(x)
```

Arguments

x [\(mlr3::ResampleResult | mlr3::BenchmarkResult\)](#).

Value

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

Data structure

The returned data table has the following columns:

- `experiment` (`integer(1)`)
Index, giving the according row number in the original benchmark grid.
- `iteration` (`integer(1)`)
Iteration of the outer resampling.
- One column for each feature of the task.
- One column for each performance measure.
- `features` (`character()`)
Vector of selected feature set.
- `task_id` (`character(1)`).
- `learner_id` (`character(1)`).
- `resampling_id` (`character(1)`).

Examples

```

at = auto_fselector(
  method = "random_search",
  learner = lrn("classif.rpart"),
  resampling = rsmpl("holdout"),
  measure = msr("classif.ce"),
  term_evals = 4)

resampling_outer = rsmpl("cv", folds = 2)
rr = resample(tsk("iris"), at, resampling_outer, store_models = TRUE)

extract_inner_fselect_results(rr)

```

fs

*Syntactic Sugar for FSelect Construction***Description**

This function complements [mlr_fselectors](#) with functions in the spirit of [mlr3::mlr_sugar](#).

Usage

```

fs(.key, ...)

fss(.keys, ...)

```

Arguments

<code>.key</code>	(character(1)) Key passed to the respective dictionary to retrieve the object.
<code>...</code>	(named list()) Named arguments passed to the constructor, to be set as parameters in the paradox::ParamSet , or to be set as public field. See mlr3misc::dictionary_sugar_get() for more details.
<code>.keys</code>	(character()) Keys passed to the respective dictionary to retrieve multiple objects.

Value

[FSelector](#).

Examples

```

fs("sequential", max_features = 4)

```

fselect *Function for Feature Selection*

Description

Function to optimize the feature set of a [mlr3::Learner](#).

Usage

```
fselect(  
  method,  
  task,  
  learner,  
  resampling,  
  measure,  
  term_evals = NULL,  
  term_time = NULL,  
  ...  
)
```

Arguments

method	(character(1)) Key to retrieve fselector from mlr_fselectors dictionary.
task	(mlr3::Task) Task to operate on.
learner	(mlr3::Learner).
resampling	(mlr3::Resampling) Uninstantiated resamplings are instantiated during construction so that all configurations are evaluated on the same data splits.
measure	(mlr3::Measure) Measure to optimize.
term_evals	(integer(1)) Number of allowed evaluations.
term_time	(integer(1)) Maximum allowed time in seconds.
...	(named list()) Named arguments to be set as parameters of the fselector.

Value

FSelectInstanceSingleCrit

Examples

```

task = tsk("pima")

instance = fselect(
  method = "random_search",
  task = task,
  learner = lrn("classif.rpart"),
  resampling = rsmp("holdout"),
  measure = msr("classif.ce"),
  term_evals = 4)

# subset task to optimized feature set
task$select(instance$result_feature_set)

```

FSelectInstanceMultiCrit

Multi Criterion Feature Selection Instance

Description

Specifies a general feature selection scenario, including objective function and archive for feature selection algorithms to act upon. This class stores an [ObjectiveFSelect](#) object that encodes the black box objective function which an [FSelector](#) has to optimize. It allows the basic operations of querying the objective at feature subsets (`$eval_batch()`), storing the evaluations in the internal [bbotk::Archive](#) and accessing the final result (`$result`).

Evaluations of feature subsets are performed in batches by calling `mlr3::benchmark()` internally. Before a batch is evaluated, the [bbotk::Terminator](#) is queried for the remaining budget. If the available budget is exhausted, an exception is raised, and no further evaluations can be performed from this point on.

The [FSelector](#) is also supposed to store its final result, consisting of the selected feature subsets and associated estimated performance values, by calling the method `instance$assign_result()`.

Super classes

```
bbotk::OptimInstance -> bbotk::OptimInstanceMultiCrit -> FSelectInstanceMultiCrit
```

Active bindings

```
result_feature_set (list() of character())
  Feature sets for task subsetting.
```

Methods**Public methods:**

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

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

Usage:

```
FSelectInstanceMultiCrit$new(
  task,
  learner,
  resampling,
  measures,
  terminator,
  store_models = FALSE,
  check_values = TRUE,
  store_benchmark_result = TRUE
)
```

Arguments:

`task` (`mlr3::Task`)

Task to operate on.

`learner` (`mlr3::Learner`).

`resampling` (`mlr3::Resampling`)

Uninstantiated resamplings are instantiated during construction so that all configurations are evaluated on the same data splits.

`measures` (list of `mlr3::Measure`)

Measures to optimize. If NULL, `mlr3`'s default measure is used.

`terminator` (`bbotk::Terminator`).

`store_models` (`logical(1)`). Store models in benchmark result?

`check_values` (`logical(1)`)

Check the parameters before the evaluation and the results for validity?

`store_benchmark_result` (`logical(1)`)

Store benchmark result in archive?

Method `assign_result()`: The `FSelector` object writes the best found feature subsets and estimated performance values here. For internal use.

Usage:

```
FSelectInstanceMultiCrit$assign_result(xdt, ydt)
```

Arguments:

`xdt` (`data.table::data.table()`)

x values as `data.table`. Each row is one point. Contains the value in the *search space* of the `FSelectInstanceMultiCrit` object. Can contain additional columns for extra information.

`ydt` (`data.table::data.table()`)

Optimal outcomes, e.g. the Pareto front.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Examples

```

library(mlr3)
library(data.table)

# Objects required to define the performance evaluator
task = tsk("iris")
measures = msrs(c("classif.ce", "classif.acc"))
learner = lrn("classif.rpart")
resampling = rsmp("cv")
terminator = trm("evals", n_evals = 8)

inst = FSelectInstanceMultiCrit$new(
  task = task,
  learner = learner,
  resampling = resampling,
  measures = measures,
  terminator = terminator
)

# Try some feature subsets
xdt = data.table(
  Petal.Length = c(TRUE, FALSE),
  Petal.Width = c(FALSE, TRUE),
  Sepal.Length = c(TRUE, FALSE),
  Sepal.Width = c(FALSE, TRUE)
)

inst$eval_batch(xdt)

# Get archive data
as.data.table(inst$archive)

```

FSelectInstanceSingleCrit

Single Criterion Feature Selection Instance

Description

Specifies a general feature selection scenario, including objective function and archive for feature selection algorithms to act upon. This class stores an [ObjectiveFSelect](#) object that encodes the black box objective function which an [FSelector](#) has to optimize. It allows the basic operations of querying the objective at feature subsets (`$eval_batch()`), storing the evaluations in the internal [bbotk::Archive](#) and accessing the final result (`$result`).

Evaluations of feature subsets are performed in batches by calling `mlr3::benchmark()` internally. Before a batch is evaluated, the [bbotk::Terminator](#) is queried for the remaining budget. If the available budget is exhausted, an exception is raised, and no further evaluations can be performed from this point on.

The [FSelector](#) is also supposed to store its final result, consisting of a selected feature subset and associated estimated performance values, by calling the method `instance$assign_result()`.

Super classes

`bbotk::OptimInstance -> bbotk::OptimInstanceSingleCrit -> FSelectInstanceSingleCrit`

Active bindings

`result_feature_set` (`character()`)
Feature set for task subsetting.

Methods**Public methods:**

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

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

Usage:

```
FSelectInstanceSingleCrit$new(
  task,
  learner,
  resampling,
  measure,
  terminator,
  store_models = FALSE,
  check_values = TRUE,
  store_benchmark_result = TRUE
)
```

Arguments:

`task` (`mlr3::Task`)

Task to operate on.

`learner` (`mlr3::Learner`).

`resampling` (`mlr3::Resampling`)

Uninstantiated resamplings are instantiated during construction so that all configurations are evaluated on the same data splits.

`measure` (`mlr3::Measure`)

Measure to optimize.

`terminator` (`bbotk::Terminator`).

`store_models` (`logical(1)`). Store models in benchmark result?

`check_values` (`logical(1)`)

Check the parameters before the evaluation and the results for validity?

`store_benchmark_result` (`logical(1)`)

Store benchmark result in archive?

Method `assign_result()`: The `FSelector` writes the best found feature subset and estimated performance value here. For internal use.

Usage:

```
FSelectInstanceSingleCrit$assign_result(xdt, y)
```

Arguments:

```
xdt (data.table::data.table())
```

x values as `data.table`. Each row is one point. Contains the value in the *search space* of the `FSelectInstanceMultiCrit` object. Can contain additional columns for extra information.

```
y (numeric(1))
```

Optimal outcome.

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Examples

```
library(mlr3)
library(data.table)

# Objects required to define the objective function
task = tsk("iris")
measure = msr("classif.ce")
learner = lrn("classif.rpart")
resampling = rsmp("cv")

# Create instance
terminator = trm("evals", n_evals = 8)
inst = FSelectInstanceSingleCrit$new(
  task = task,
  learner = learner,
  resampling = resampling,
  measure = measure,
  terminator = terminator
)

# Try some feature subsets
xdt = data.table(
  Petal.Length = c(TRUE, FALSE),
  Petal.Width = c(FALSE, TRUE),
  Sepal.Length = c(TRUE, FALSE),
  Sepal.Width = c(FALSE, TRUE)
)

inst$eval_batch(xdt)

# Get archive data
as.data.table(inst$archive)
```

FSelector

FSelector

Description

Abstract FSelector class that implements the base functionality each fselector must provide. A FSelector object describes the feature selection strategy, i.e. how to optimize the black-box function and its feasible set defined by the [FSelectInstanceSingleCrit](#) / [FSelectInstanceMultiCrit](#) object.

A fselector must write its result into the [FSelectInstanceSingleCrit](#) / [FSelectInstanceMultiCrit](#) using the `assign_result` method of the [bbotk::OptimInstance](#) at the end of its selection in order to store the best selected feature subset and its estimated performance vector.

Private Methods

- `.optimize(instance) -> NULL`
Abstract base method. Implement to specify feature selection of your subclass. See technical details sections.
- `.assign_result(instance) -> NULL`
Abstract base method. Implement to specify how the final feature subset is selected. See technical details sections.

Technical Details and Subclasses

A subclass is implemented in the following way:

- Inherit from FSelector.
- Specify the private abstract method `$.optimize()` and use it to call into your optimizer.
- You need to call `instance$eval_batch()` to evaluate feature subsets.
- The batch evaluation is requested at the [FSelectInstanceSingleCrit](#) / [FSelectInstanceMultiCrit](#) object `instance`, so each batch is possibly executed in parallel via `mlr3::benchmark()`, and all evaluations are stored inside of `instance$archive`.
- Before the batch evaluation, the [bbotk::Terminator](#) is checked, and if it is positive, an exception of class "terminated_error" is generated. In the later case the current batch of evaluations is still stored in `instance`, but the numeric scores are not sent back to the handling optimizer as it has lost execution control.
- After such an exception was caught we select the best feature subset from `instance$archive` and return it.
- Note that therefore more points than specified by the [bbotk::Terminator](#) may be evaluated, as the Terminator is only checked before a batch evaluation, and not in-between evaluation in a batch. How many more depends on the setting of the batch size.
- Overwrite the private super-method `.assign_result()` if you want to decide yourself how to estimate the final feature subset in the instance and its estimated performance. The default behavior is: We pick the best resample-experiment, regarding the given measure, then assign its feature subset and aggregated performance to the instance.

Public fields

param_set ([paradox::ParamSet](#)).
 param_classes (character()).
 properties (character()).
 packages (character()).

Methods**Public methods:**

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

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

Usage:

```
FSelector$new(param_set, properties, packages = character(0))
```

Arguments:

param_set [paradox::ParamSet](#)

Set of control parameters for fselector.

properties (character())

Set of properties of the fselector. Must be a subset of [mlr_reflections\\$fselect_properties](#).

packages (character())

Set of required packages. Note that these packages will be loaded via [requireNamespace\(\)](#), and are not attached.

Method [format\(\)](#): Helper for print outputs.

Usage:

```
FSelector$format()
```

Returns: (character()).

Method [print\(\)](#): Print method.

Usage:

```
FSelector$print()
```

Returns: (character()).

Method [optimize\(\)](#): Performs the feature selection on a [FSelectInstanceSingleCrit](#) or [FSelectInstanceMultiCrit](#) until termination. The single evaluations will be written into the [ArchiveFSelect](#) that resides in the [FSelectInstanceSingleCrit](#) / [FSelectInstanceMultiCrit](#). The result will be written into the instance object.

Usage:

```
FSelector$optimize(inst)
```

Arguments:

inst (FSelectInstanceSingleCrit|FSelectInstanceMultiCrit).

Returns: data.table::data.table.

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

Usage:

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

Arguments:

deep Whether to make a deep clone.

Examples

```
library(mlr3)

terminator = trm("evals", n_evals = 3)

instance = FSelectInstanceSingleCrit$new(
  task = tsk("iris"),
  learner = lrn("classif.rpart"),
  resampling = rsmpl("holdout"),
  measure = msr("classif.ce"),
  terminator = terminator
)

# swap this line to use a different FSelector
fselector = fs("random_search")

# modifies the instance by reference
fselector$optimize(instance)

# returns best feature subset and best performance
instance$result

# allows access of data.table / benchmark result of full path of all evaluations
instance$archive
```

FSelectorDesignPoints *Feature Selection via Design Points*

Description

FSelectorDesignPoints class that implements feature selection w.r.t. fixed feature sets. We simply search over a set of feature subsets fully specified by the user. The feature sets are evaluated in order as given.

In order to support general termination criteria and parallelization, we evaluate feature sets in a batch-fashion of size `batch_size`. Larger batches mean we can parallelize more, smaller batches imply a more fine-grained checking of termination criteria.

Dictionary

This `FSelector` can be instantiated via the dictionary `mlr_fselectors` or with the associated sugar function `fs()`:

```
mlr_fselectors$get("design_points")
fs("design_points")
```

Parameters

`batch_size` integer(1)
Maximum number of configurations to try in a batch.

`design` `data.table::data.table`
Design points to try in search, one per row.

Super classes

```
mlr3fselect::FSelector -> mlr3fselect::FSelectorFromOptimizer -> FSelectorDesignPoints
```

Methods**Public methods:**

- `FSelectorDesignPoints$new()`
- `FSelectorDesignPoints$clone()`

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

Usage:

```
FSelectorDesignPoints$new()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Examples

```
library(mlr3)
library(data.table)

terminator = trm("evals", n_evals = 10)

instance = FSelectInstanceSingleCrit$new(
  task = tsk("iris"),
  learner = lrn("classif.rpart"),
  resampling = rsmp("holdout"),
  measure = msr("classif.ce"),
  terminator = terminator
)
```

```

design = data.table(Petal.Length = c(TRUE, FALSE),
  Petal.Width = c(TRUE, FALSE),
  Sepal.Length = c(FALSE, TRUE),
  Sepal.Width = c(FALSE, TRUE))

fselector = fs("design_points", design = design)

# Modifies the instance by reference
fselector$optimize(instance)

# Returns best scoring evaluation
instance$result

# Allows access of data.table of full path of all evaluations
as.data.table(instance$archive)

```

FSelectorExhaustiveSearch

Feature Selection via Exhaustive Search

Description

FSelectorExhaustiveSearch class that implements an Exhaustive Search.

In order to support general termination criteria and parallelization, feature sets are evaluated in batches. The size of the feature sets is increased by 1 in each batch.

Dictionary

This [FSelector](#) can be instantiated via the [dictionary mlr_fselectors](#) or with the associated sugar function `fs()`:

```

mlr_fselectors$get("exhaustive_search")
fs("exhaustive_search")

```

Parameters

`max_features` integer(1)
Maximum number of features. By default, number of features in [mlr3::Task](#).

Super class

[mlr3fselect::FSelector](#) -> FSelectorExhaustiveSearch

Methods

Public methods:

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

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

Usage:

```
FSelectorExhaustiveSearch$new()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Examples

```
library(mlr3)

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

instance = FSelectInstanceSingleCrit$new(
  task = tsk("iris"),
  learner = lrn("classif.rpart"),
  resampling = rsmpl("holdout"),
  measure = msr("classif.ce"),
  terminator = terminator
)

fselector = fs("exhaustive_search")

# Modifies the instance by reference
fselector$optimize(instance)

# Returns best scoring evaluation
instance$result

# Allows access of data.table of full path of all evaluations
as.data.table(instance$archive)
```

FSelectorGeneticSearch

Feature Selection via Genetic Search

Description

FSelectorGeneticSearch class that implements an Genetic Search. Calls `genalg::rbga.bin()` from package **genalg**.

Dictionary

This `FSelector` can be instantiated via the dictionary `mlr_fselectors` or with the associated sugar function `fs()`:

```
mlr_fselectors$get("genetic_search")
fs("genetic_search")
```

Parameters

```
suggestions list()
popSize integer(1)
mutationChance numeric(1)
elitism integer(1)
zeroToOneRatio integer(1)
iters integer(1)
```

For the meaning of the control parameters, see `genalg::rbga.bin()`. `genalg::rbga.bin()` internally terminates after `iters` iteration. We set `iters = 100000` to allow the termination via our terminators. If more iterations are needed, set `iters` to a higher value in the parameter set.

Super class

```
mlr3fselect::FSelector -> FSelectorGeneticSearch
```

Methods

Public methods:

- `FSelectorGeneticSearch$new()`
- `FSelectorGeneticSearch$clone()`

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

Usage:

```
FSelectorGeneticSearch$new()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Examples

```

library(mlr3)

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

instance = FSelectInstanceSingleCrit$new(
  task = tsk("iris"),
  learner = lrn("classif.rpart"),
  resampling = rsmp("holdout"),
  measure = msr("classif.ce"),
  terminator = terminator
)

fselector = fs("genetic_search", popSize = 10L)

# Modifies the instance by reference
fselector$optimize(instance)

# Returns best scoring evaluation
instance$result

# Allows access of data.table of full path of all evaluations
as.data.table(instance$archive)

```

FSelectorRandomSearch *Feature Selection via Random Search*

Description

FSelectorRandomSearch class that implements a simple Random Search.

In order to support general termination criteria and parallelization, we evaluate feature sets in a batch-fashion of size `batch_size`. Larger batches mean we can parallelize more, smaller batches imply a more fine-grained checking of termination criteria.

Dictionary

This [FSelector](#) can be instantiated via the [dictionary mlr_fselectors](#) or with the associated sugar function `fs()`:

```

mlr_fselectors$get("random_search")
fs("random_search")

```

Parameters

`max_features` integer(1)
 Maximum number of features. By default, number of features in [mlr3::Task](#).

`batch_size` integer(1)
 Maximum number of feature sets to try in a batch.

Super class

```
mlr3fselect::FSelector -> FSelectorRandomSearch
```

Methods**Public methods:**

- `FSelectorRandomSearch$new()`
- `FSelectorRandomSearch$clone()`

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

Usage:

```
FSelectorRandomSearch$new()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Source

Bergstra J, Bengio Y (2012). “Random Search for Hyper-Parameter Optimization.” *Journal of Machine Learning Research*, **13**(10), 281–305. <https://jmlr.csail.mit.edu/papers/v13/bergstra12a.html>.

Examples

```
library(mlr3)

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

instance = FSelectInstanceSingleCrit$new(
  task = tsk("iris"),
  learner = lrn("classif.rpart"),
  resampling = rsm("holdout"),
  measure = msr("classif.ce"),
  terminator = terminator
)

fselector = fs("random_search")

# Modifies the instance by reference
fselector$optimize(instance)

# Returns best scoring evaluation
instance$result

# Allows access of data.table of full path of all evaluations
as.data.table(instance$archive)
```

Description

FSelectorRFE class that implements Recursive Feature Elimination (RFE). The recursive algorithm (`recursive = TRUE`) recomputes the feature importance on the reduced feature set in every iteration. The non-recursive algorithm (`recursive = FALSE`) only uses the feature importance of the model fitted with all features to eliminate the next most unimportant features in every iteration.

Dictionary

This [FSelector](#) can be instantiated via the [dictionary mlr_fselectors](#) or with the associated sugar function `fs()`:

```
mlr_fselectors$get("rfe")  
fs("rfe")
```

Parameters

`min_features` integer(1)

The minimum number of features to select, default is 1L.

`feature_fraction` double(1)

Fraction of features to retain in each iteration, default is 0.5.

`feature_number` integer(1)

Number of features to remove in each iteration.

`subset_sizes` integer()

Vector of number of features to retain in each iteration. Must be sorted in decreasing order.

`recursive` logical(1)

Use the recursive version? Default is FALSE.

The parameter `feature_fraction`, `feature_number` and `subset_sizes` are mutually exclusive.

Super class

```
mlr3fselect::FSelector -> FSelectorRFE
```

Public fields

`importance` numeric()

Stores the feature importance of the model with all variables if recursive is set to FALSE

Methods

Public methods:

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

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

Usage:

```
FSelectorRFE$new()
```

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Examples

```
library(mlr3)

terminator = trm("evals", n_evals = 10)
instance = FSelectInstanceSingleCrit$new(
  task = tsk("iris"),
  learner = lrn("classif.rpart"),
  resampling = rsmpl("holdout"),
  measure = msr("classif.ce"),
  terminator = terminator,
  store_models = TRUE
)

fselector = fs("rfe")

# Modifies the instance by reference
fselector$optimize(instance)

# Returns best scoring evaluation
instance$result

# Allows access of data.table of full path of all evaluations
as.data.table(instance$archive)
```

Description

FSelectorSequential class that implements sequential feature selection. The sequential forward selection (strategy = fsf) extends the feature set in each step with the feature that increases the models performance the most. The sequential backward selection (strategy = fsb) starts with the complete feature set and removes in each step the feature that decreases the models performance the least.

Dictionary

This FSelector can be instantiated via the dictionary `mlr_fselectors` or with the associated sugar function `fs()`:

```
mlr_fselectors$get("sequential")
fs("sequential")
```

Parameters

`max_features` integer(1)
Maximum number of features. By default, number of features in `mlr3::Task`.

`strategy` character(1)
Search method sfs (forward search) or sbs (backward search).

Super class

```
mlr3fselect::FSelector -> FSelectorSequential
```

Methods**Public methods:**

- `FSelectorSequential$new()`
- `FSelectorSequential$optimization_path()`
- `FSelectorSequential$clone()`

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

Usage:

```
FSelectorSequential$new()
```

Method `optimization_path()`: Returns the optimization path.

Usage:

```
FSelectorSequential$optimization_path(inst, include_uhash = FALSE)
```

Arguments:

`inst` (`FSelectInstanceSingleCrit`)
Instance optimized with `FSelectorSequential`.

`include_uhash` (logical(1))
Include uhash column?

Returns: `data.table::data.table()`

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

Usage:

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

Arguments:

deep Whether to make a deep clone.

Note

Feature sets are evaluated in batches, where each batch is one step in the sequential feature selection.

Examples

```
library(mlr3)

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

instance = FSelectInstanceSingleCrit$new(
  task = tsk("iris"),
  learner = lrn("classif.rpart"),
  resampling = rsm("holdout"),
  measure = msr("classif.ce"),
  terminator = terminator
)

fselector = fs("sequential")

# Modifies the instance by reference
fselector$optimize(instance)

# Returns best scoring evaluation
instance$result

# Allows access of data.table of full path of all evaluations
as.data.table(instance$archive)
```

FSelectorShadowVariableSearch

Feature Selection via Sequential Search with Shadow Variables

Description

FSelectorShadowVariableSearch class that implements a sequential search with shadow variables.

Dictionary

This `FSelector` can be instantiated via the dictionary `mlr_fselectors` or with the associated sugar function `fs()`:

```
mlr_fselectors$get("shadow_variable_search")
fs("shadow_variable_search")
```

Super class

```
mlr3fselect::FSelector -> FSelectorShadowVariableSearch
```

Methods**Public methods:**

- `FSelectorShadowVariableSearch$new()`
- `FSelectorShadowVariableSearch$optimization_path()`
- `FSelectorShadowVariableSearch$clone()`

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

Usage:

```
FSelectorShadowVariableSearch$new()
```

Method `optimization_path()`: Returns the optimization path.

Usage:

```
FSelectorShadowVariableSearch$optimization_path(inst)
```

Arguments:

`inst` (`FSelectInstanceSingleCrit`)

Instance optimized with `FSelectorShadowVariableSearch`.

Returns: `data.table::data.table`

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

Usage:

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

Arguments:

`deep` Whether to make a deep clone.

Note

`FSelectorShadowVariableSearch` terminates itself and should be used with `TerminatorNone`.

Source

Thomas J, Hepp T, Mayr A, Bischl B (2017). “Probing for Sparse and Fast Variable Selection with Model-Based Boosting.” *Computational and Mathematical Methods in Medicine*, **2017**, 1–8. doi: [10.1155/2017/1421409](https://doi.org/10.1155/2017/1421409). Wu Y, Boos DD, Stefanski LA (2007). “Controlling Variable Selection by the Addition of Pseudovariabes.” *Journal of the American Statistical Association*, **102**(477), 235–243. doi: [10.1198/016214506000000843](https://doi.org/10.1198/016214506000000843).

Examples

```

library(mlr3)

instance = FSelectInstanceSingleCrit$new(
  task = tsk("iris"),
  learner = lrn("classif.rpart"),
  resampling = rsmpl("holdout"),
  measure = msr("classif.ce"),
  terminator = trm("none")
)

fselector = fs("shadow_variable_search")

# Modifies the instance by reference
fselector$optimize(instance)

# Returns best scoring evaluation
instance$result

# Allows access of data.table of full path of all evaluations
as.data.table(instance$archive)

```

fselect_nested

Function for Nested Resampling

Description

Function to conduct nested resampling.

Usage

```

fselect_nested(
  method,
  task,
  learner,
  inner_resampling,
  outer_resampling,
  measure,
  term_evals = NULL,
  term_time = NULL,
  ...
)

```

Arguments

method (character(1))
Key to retrieve fselector from [mlr_fselectors](#) dictionary.

task	(mlr3::Task) Task to operate on.
learner	(mlr3::Learner).
inner_resampling	(mlr3::Resampling) Resampling used for the inner loop.
outer_resampling	mlr3::Resampling Resampling used for the outer loop.
measure	(mlr3::Measure) Measure to optimize.
term_evals	(integer(1)) Number of allowed evaluations.
term_time	(integer(1)) Maximum allowed time in seconds.
...	(named list()) Named arguments to be set as parameters of the fselector.

Value

mlr3::ResampleResult

Examples

```
rr = fselect_nested(
  method = "random_search",
  task = tsk("pima"),
  learner = lrn("classif.rpart"),
  inner_resampling = rsmpl("holdout"),
  outer_resampling = rsmpl("cv", folds = 2),
  measure = msr("classif.ce"),
  term_evals = 4)

# performance scores estimated on the outer resampling
rr$score()

# unbiased performance of the final model trained on the full data set
rr$aggregate()
```

mlr_fselectors

mlr_fselectors

Description

A `mlr3misc::Dictionary` storing objects of class `FSelector`.

Usage

```
mlr_fselectors
```

Format

An object of class DictionaryFSelect (inherits from Dictionary, R6) of length 13.

```
ObjectiveFSelect      ObjectiveFSelect
```

Description

Stores the objective function that estimates the performance of feature subsets. This class is usually constructed internally by the [FSelectInstanceSingleCrit](#) / [FSelectInstanceMultiCrit](#).

Super class

```
bbotk::Objective -> ObjectiveFSelect
```

Public fields

```
task (mlr3::Task)
learner (mlr3::Learner)
resampling (mlr3::Resampling)
measures (list of mlr3::Measure)
store_models (logical(1)).
store_benchmark_result (logical(1)).
archive (ArchiveFSelect).
```

Methods**Public methods:**

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

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

Creates a new instance of this R6 class.

Usage:

```
ObjectiveFSelect$new(
  task,
  learner,
  resampling,
  measures,
  check_values = TRUE,
  store_benchmark_result = TRUE,
  store_models = FALSE
)
```

Arguments:

task ([mlr3::Task](#))

Task to operate on.

learner ([mlr3::Learner](#)).

resampling ([mlr3::Resampling](#))

Uninstantiated resamplings are instantiated during construction so that all configurations are evaluated on the same data splits.

measures (list of [mlr3::Measure](#))

Measures to optimize. If NULL, **mlr3**'s default measure is used.

check_values (logical(1))

Check the parameters before the evaluation and the results for validity?

store_benchmark_result (logical(1))

Store benchmark result in archive?

store_models (logical(1)). Store models in benchmark result?

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

Usage:

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

Arguments:

deep Whether to make a deep clone.

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