

Package ‘flowml’

July 22, 2025

Type Package

Title A Backend for a 'nextflow' Pipeline that Performs
Machine-Learning-Based Modeling of Biomedical Data

Version 0.1.3

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Description

Provides functionality to perform machine-learning-based modeling in a computation pipeline. Its functions contain the basic steps of machine-learning-based knowledge discovery workflows, including model training and optimization, model evaluation, and model testing. To perform these tasks, the package builds heavily on existing machine-learning packages, such as 'caret' <<https://github.com/topepo/caret/>> and associated packages. The package can train multiple models, optimize model hyperparameters by performing a grid search or a random search, and evaluates model performance by different metrics. Models can be validated either on a test data set, or in case of a small sample size by k-fold cross validation or repeated bootstrapping. It also allows for 0-Hypotheses generation by performing permutation experiments. Additionally, it offers methods of model interpretation and item categorization to identify the most informative features from a high dimensional data space. The functions of this package can easily be integrated into computation pipelines (e.g. 'nextflow' <<https://www.nextflow.io/>>) and hereby improve scalability, standardization, and re-productibility in the context of machine-learning.

License GPL (>= 3)

Encoding UTF-8

URL <https://github.com/Boehringer-Ingelheim/flowml>

BugReports <https://github.com/Boehringer-Ingelheim/flowml/issues>

Imports ABCanalysis, caret, data.table, dplyr, fastshap, furr,
future, magrittr, optparse, parallel, purrr, R6, readr, rjson,
rlang, rsample, stats, stringr, tibble, tidyr, utils, vip

RoxyenNote 7.2.3

Collate 'fml_resampler.R' 'fml_resample.R' 'fml_format_response.R'
'fml_parser.R' 'fml_bootstrap.R' 'fml_categorize.R'

```
'fml_example.R' 'fml_globals.R' 'fml_grids.R' 'fml_interpret.R'
'fml_train.R' 'fml_validate.R'
```

Suggests ada, adabag, arm, bartMachine, bst, C50, caTools, class, Cubist, e1071, earth, elasticnet, evtree, fastICA, foreach, frbs, gam, gbm, ggplot2, glmnet, h2o, hda, ipred, keras, kernlab, kknn, klaR, knitr, kohonen, lars, leaps, LiblineaR, LogicReg, MASS, Matrix, mboost, mda, mgcv, monomvn, neuralnet, nnet, nnls, pamr, partDSA, party, partykit, penalized, pls, plyr, proxy, quantregForest, randomForest, ranger, rFerns, rmarkdown, rpart, rrcov, rrcovHD, RSNNS, RWeka, sda, shapviz, spls, superpc, VGAM, xgboost

Depends R (>= 3.5.0)

NeedsCompilation no

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Repository CRAN

Date/Publication 2024-02-16 10:40:02 UTC

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create_parser	<i>create_parser</i>
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Description

Creates an object that defines and handles command line arguments.

Usage

```
create_parser()
```

Details

A parser that organizes the communication between the user and the function. It also provides a help message.

Value

An instance of type 'optparse::OptionParser'.

Author(s)

Sebastian Malkusch

```
create_resample_experiment
```

create_resample_experiment

Description

Creates an object of a resampling experiment.

Usage

```
create_resample_experiment(  
  seed,  
  data_df,  
  parser_inst,  
  model_inst,  
  config_inst,  
  n_features  
)
```

Arguments

seed	sets the seed for the random number generator to guarantee reproducibility. (int)
data_df	data frame to be learned from. (tibble::tibble)
parser_inst	instance of parser object. (optparse::parse_args).
model_inst	instance of caret_train object (caret::train).
config_inst	list of config options (list).
n_features	number of features (int).

Details

Creates a resampling experiment. It uses user defined parameters to set up the experiment. It creates an instance of the Resampler object and runs the experiment according to the user-defined parameters.

Value

An instance of type 'Resampler'.

Author(s)

Sebastian Malkusch

fml_bootstrap

fml_bootstrap

Description

Pipeline function that sets up and runs a resampling experiment.

Usage

```
fml_bootstrap(parser_inst)
```

Arguments

parser_inst Instance of fml_parser class that comprises command line arguments.

Details

The experiment is run in parallel. All results are written to files.

Value

none

Author(s)

Sebastian Malkusch

Examples

```
## Not run:
parser_inst <- flowml::create_parser()

parser_inst$pipeline_segment <- "bootstrap"
parser_inst$config <- flowml::fml_example(file = "reg_config.json")
parser_inst$data <- flowml::fml_example(file = "reg_data.csv")
parser_inst$samples_train <- flowml::fml_example(file = "reg_samples_train.txt")
parser_inst$samples_test <- flowml::fml_example(file = "reg_samples_test.txt")
parser_inst$features <- flowml::fml_example(file = "reg_features.txt")
parser_inst$extended_features <- flowml::fml_example(file = "reg_features_extended.txt")
parser_inst$trained <- flowml::fml_example(file = "reg_fit.rds")
parser_inst$permutation <- "none"
parser_inst$result_dir <- tempdir()

flowml::fml_bootstrap(parser_inst = parser_inst)

## End(Not run)
```

fml_example

*fml_example***Description**

path to flowml examples data

Usage

```
fml_example(file = NULL)
```

Arguments

file Name of file. If 'NULL', the example files will be listed.

Details

flowml comes bundled with a number of sample files in its 'inst/extdata' directory. This function allows to access them.

Value

The path of to an example file, if file is defined. Else, a list of example files.

Author(s)

Sebastian Malkusch

Examples

```
## Not run:
fml_example()
fml_example(file = "reg_config.json")

## End(Not run)
```

fml_interpret

*fml_interpret***Description**

Pipeline function that sets up and runs a post-hoc interpretation of an ml experiment. All results are written to rds files.

Usage

```
fml_interpret(parser_inst)
```

Arguments

parser_inst instance of fml_parser class that comprises command line arguments.

Value

none

Author(s)

Sebastian Malkusch

Examples

```
## Not run:
parser_inst <- flowml::create_parser()

parser_inst$pipeline_segment <- "interpret"
parser_inst$config <- flowml::fml_example(file = "reg_config.json")
parser_inst$data <- flowml::fml_example(file = "reg_data.csv")
parser_inst$samples_train <- flowml::fml_example(file = "reg_samples_train.txt")
parser_inst$samples_test <- flowml::fml_example(file = "reg_samples_test.txt")
parser_inst$features <- flowml::fml_example(file = "reg_features.txt")
parser_inst$extended_features <- flowml::fml_example(file = "reg_features_extended.txt")
parser_inst$trained <- flowml::fml_example(file = "reg_fit.rds")
parser_inst$interpretation <- "shap"
parser_inst$result_dir <- tempdir()

flowml::fml_interpret(parser_inst = parser_inst)
```

```
## End(Not run)
```

fml_train

fml_train

Description

Pipeline function that performs a hyper-parameter screeing experiment.

Usage

```
fml_train(parser_inst)
```

Arguments

parser_inst instance of fml_parser class that comprises command line arguments.

Value

none

Author(s)

Kolja Becker

Examples

```
## Not run:
parser_inst <- flowml::create_parser()

parser_inst$pipeline_segment <- "train"
parser_inst$config <- flowml::fml_example(file = "reg_config.json")
parser_inst$data <- flowml::fml_example(file = "reg_data.csv")
parser_inst$samples_train <- flowml::fml_example(file = "reg_samples_train.txt")
parser_inst$samples_test <- flowml::fml_example(file = "reg_samples_test.txt")
parser_inst$features <- flowml::fml_example(file = "reg_features.txt")
parser_inst$extended_features <- flowml::fml_example(file = "reg_features_extended.txt")
parser_inst$result_dir <- tempdir()

flowml::fml_train(parser_inst = parser_inst)

## End(Not run)
```

fml_validate	<i>fml_validate</i>
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Description

Pipeline function that performs a validation experiment on a a caret train object based on test samples.

Usage

```
fml_validate(parser_inst)
```

Arguments

`parser_inst` instance of `fml_parser` class that comprises command line arguments.

Value

none

Author(s)

Kolja Becker

Examples

```
## Not run:
parser_inst <- flowml::create_parser()

parser_inst$pipeline_segment <- "validate"
parser_inst$config <- flowml::fml_example(file = "reg_config.json")
parser_inst$data <- flowml::fml_example(file = "reg_data.csv")
parser_inst$samples_train <- flowml::fml_example(file = "reg_samples_train.txt")
parser_inst$samples_test <- flowml::fml_example(file = "reg_samples_test.txt")
parser_inst$features <- flowml::fml_example(file = "reg_features.txt")
parser_inst$extended_features <- flowml::fml_example(file = "reg_features_extended.txt")
parser_inst$trained <- flowml::fml_example(file = "reg_fit.rds")
parser_inst$permutation <- "none"
parser_inst$result_dir <- tempdir()

flowml::fml_validate(parser_inst = parser_inst)

## End(Not run)
```

format_y	<i>format_y</i>
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Description

Formats response variable based on the ml-type variable passed by the config file. For regression analyses the response variable will be explicitly transformed to type numeric. For Classification experiments the response variable will be explicitly transformed to a factor. Time-to-event models are to be implemented in the near future.

Usage

```
format_y(y, ml.type)
```

Arguments

y	vector of response variable.
ml.type	type of experiment (character).

Value

a transformed version of the response variable y.

Author(s)

Kolja Becker

Resampler	<i>Resampler</i>
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Description

Model validation by repeated bootstrapping

Format

[R6::R6Class] object.

Details

Uses repeated bootstrapping to validate models without a test data set. For each experiment multiple metrics are measured. For classification experiments the confusion matrix is calculated additionally. In order to test hypotheses, either features or the response variable can be permuted.

Active bindings

`permute` returns the instance variable `'permute'`. (character)
`permute_alphabet` returns the instance variable `'permute_alphabet'`. (character)
`n_resample` returns the instance variable `'n_resample'`. (integer)
`fml_method` returns the instance variable `'fml_method'`. (character)
`fml_type` returns the instance variable `'fml_type'`. (character)
`fml_type_alphabet` returns the instance variable `'fml_type_alphabet'`. (character)
`pre_process_lst` returns the instance variable `'pre_process_lst'`. (character)
`hyper_parameters` returns the instance variable `'hyper_parameters'`. (list)
`response_var` returns the instance variable `'response_var'`. (character)
`n_features` returns the instance variable `'n_features'`. (integer)
`strata_var` returns the instance variable `'strata_var'`. (character)
`metrics_df` returns the instance variable `'metrics_df'`. (tibble::tibble)
`confusion_df` returns the instance variable `'confusion_df'`. (tibble::tibble)

Methods**Public methods:**

- [Resampler\\$new\(\)](#)
- [Resampler\\$print\(\)](#)
- [Resampler\\$fit\(\)](#)
- [Resampler\\$clone\(\)](#)

Method `new()`: checks, if permutation is requested. If true, performs the permutation task.
 Checks if `ml.type` is classification. If true, calculates confusion matrix.
 Creates and returns instance of Resampler class.

Usage:

```

Resampler$new(
  n_resample = 500,
  fml_method = "pcr",
  fml_type = "classification",
  hyper_parameters = "list",
  pre_process_lst = c("center", "scale"),
  permute = NULL,
  n_features = 0,
  response_var = "character",
  strata_var = NULL
)

```

Arguments:

`n_resample` number of bootstrap resamples. The default is 500 (integer)
`fml_method` ML model that is being used. The default is `'pcr'` (character).
`fml_type` ML model type. Needs to be `'classification'`, `'regression'` or `'censored'`. Default is `'classification'` (character).

hyper_parameters List of model hyper parameters. (list)
pre_process_lst Vector of pre-processing steps. Default is 'c("center", "scale")' (character).
permute Permutation method. Needs to be 'none', 'features' or 'response'. (character)
n_features Number of features to be chosen in the permutation experiment. Default is 0 (integer).
response_var Response variable of the model (character).
strata_var Stratification variable (character).

Returns: Resampler

Method print(): Print instance variables of Resampler class.

Usage:

Resampler\$print()

Returns: character

Method fit(): Runs the bootstrap analysis based on the instance variables chosen under initialize.

Usage:

Resampler\$fit(data_df = "tbl_df")

Arguments:

data_df data set to be analyzed (tibble::tibble).

Returns: None

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

Usage:

Resampler\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

Author(s)

Sebastian Malkusch

run_abc_analysis	<i>Performs item categorization</i>
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Description

Performs item categorization on permutation or shap analysis object

Usage

run_abc_analysis(data_obj, method)

Arguments

<code>data_obj</code>	Results of model interpretation experiment
<code>method</code>	Method used for model interpretation (permutatopn or shap)

Details

Interpretation results are passed to the function. Based on the type of interpretation experiment the data is transformed into a uniformly structured data frame. Item categorization is performed by computed ABC analysis. The result is returned in form of a tibble.

Value

A tibble with item categories
a tibble

Author(s)

Sebastian Malkusch

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