

Package ‘mikropml’

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Title User-Friendly R Package for Supervised Machine Learning Pipelines

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URL <http://www.schlosslab.org/mikropml/>,
<https://github.com/SchlossLab/mikropml>

BugReports <https://github.com/SchlossLab/mikropml/issues>

Description An interface to build machine learning models for classification and regression problems. ‘mikropml’ implements the ML pipeline described by Topçuoğlu et al. (2020) <doi:10.1128/mBio.00434-20> with reasonable default options for data preprocessing, hyperparameter tuning, cross-validation, testing, model evaluation, and interpretation steps. See the website <<http://www.schlosslab.org/mikropml/>> for more information, documentation, and examples.

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Encoding UTF-8

LazyData true

RoxygenNote 7.1.1

Imports caret, dplyr, e1071, glmnet, kernlab, MLmetrics, randomForest, rlang, rpart, stats, utils, xgboost

Suggests doFuture, foreach, future, future.apply, ggplot2, knitr, purrr, rmarkdown, testthat, tidyr

VignetteBuilder knitr

Depends R (>= 2.10)

NeedsCompilation no

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calc_perf_metrics *Get performance metrics for test data*

Description

Get performance metrics for test data

Usage

```
calc_perf_metrics(  
  test_data,  
  trained_model,  
  outcome_colname,  
  perf_metric_function,  
  class_probs  
)
```

Arguments

test_data	Held out test data: dataframe of outcome and features.
trained_model	Trained model from <code>caret::train()</code> .
outcome_colname	Column name as a string of the outcome variable (default NULL; the first column will be chosen automatically).
perf_metric_function	Function to calculate the performance metric to be used for cross-validation and test performance. Some functions are provided by caret (see <code>caret::defaultSummary()</code>). Defaults: binary classification = <code>twoClassSummary</code> , multi-class classification = <code>multiClassSummary</code> , regression = <code>defaultSummary</code> .
class_probs	Whether to use class probabilities (TRUE for categorical outcomes, FALSE for numeric outcomes).

Value

Dataframe of performance metrics.

Author(s)

Zena Lapp, <zenalapp@umich.edu>

Examples

```
results <- run_ml(otu_small, "glmnet", kfold = 2, cv_times = 2)  
calc_perf_metrics(results$test_data,  
  results$trained_model,  
  "dx",
```

```
multiClassSummary,  
class_probs = TRUE  
)
```

combine_hp_performance

Combine hyperparameter performance metrics for multiple train/test splits

Description

Combine hyperparameter performance metrics for multiple train/test splits generated by, for instance, [looping in R](#) or using a [snakemake workflow](#) on a high-performance computer.

Usage

```
combine_hp_performance(trained_model_lst)
```

Arguments

```
trained_model_lst  
List of trained models.
```

Value

Named list:

- dat: Dataframe of performance metric for each group of hyperparameters
- params: Hyperparameters tuned.
- Metric: Performance metric used.

Author(s)

Zena Lapp, <zenalapp@umich.edu>

Examples

```
results <- lapply(seq(100, 102), function(seed) {  
  run_ml(otu_small, "glmnet", seed = seed, cv_times = 2, kfold = 2)  
})  
models <- lapply(results, function(x) x$trained_model)  
combine_hp_performance(models)
```

`define_cv`*Define cross-validation scheme and training parameters*

Description

Define cross-validation scheme and training parameters

Usage

```
define_cv(  
  train_data,  
  outcome_colname,  
  hyperparams_list,  
  perf_metric_function,  
  class_probs,  
  kfold = 5,  
  cv_times = 100,  
  groups = NULL  
)
```

Arguments

<code>train_data</code>	Dataframe for training model.
<code>outcome_colname</code>	Column name as a string of the outcome variable (default NULL; the first column will be chosen automatically).
<code>hyperparams_list</code>	Named list of lists of hyperparameters.
<code>perf_metric_function</code>	Function to calculate the performance metric to be used for cross-validation and test performance. Some functions are provided by caret (see caret::defaultSummary()). Defaults: binary classification = <code>twoClassSummary</code> , multi-class classification = <code>multiClassSummary</code> , regression = <code>defaultSummary</code> .
<code>class_probs</code>	Whether to use class probabilities (TRUE for categorical outcomes, FALSE for numeric outcomes).
<code>kfold</code>	Fold number for k-fold cross-validation (default: 5).
<code>cv_times</code>	Number of cross-validation partitions to create (default: 100).
<code>groups</code>	Vector of groups to keep together when splitting the data into train and test sets, and for cross-validation. length matches the number of rows in the dataset (default: NULL).

Value

Caret object for `trainControl` that controls cross-validation

Author(s)

Begüm Topçuoğlu, <topcuoglu.begum@gmail.com>
Kelly Sovacool, <sovacool@umich.edu>

Examples

```
training_inds <- get_partition_indices(otu_small %>% dplyr::pull("dx"),
  training_frac = 0.8,
  groups = NULL
)
train_data <- otu_small[training_inds, ]
test_data <- otu_small[-training_inds, ]
cv <- define_cv(train_data,
  outcome_colname = "dx",
  hyperparams_list = get_hyperparams_list(otu_small, "glmnet"),
  perf_metric_function = caret::multiClassSummary,
  class_probs = TRUE,
  kfold = 5
)
```

get_caret_processed_df

Get preprocessed dataframe for continuous variables

Description

Get preprocessed dataframe for continuous variables

Usage

```
get_caret_processed_df(features, method)
```

Arguments

features	Dataframe of features for machine learning
method	Methods to preprocess the data, described in caret::preProcess() (default: c("center", "scale"), use NULL for no normalization).

Value

Named list:

- processed: Dataframe of processed features.
- removed: Names of any features removed during preprocessing.

Author(s)

Zena Lapp, <zenalapp@umich.edu>

Examples

```
get_caret_processed_df(mikropml::otu_small[, 2:ncol(otu_small)], c("center", "scale"))
```

get_corr_feats	<i>Identify correlated features</i>
----------------	-------------------------------------

Description

Identify correlated features

Usage

```
get_corr_feats(features, corr_thresh = 1, group_neg_corr = TRUE)
```

Arguments

features	Features used for machine learning.
corr_thresh	For feature importance, group correlations above or equal to corr_thresh (range 0 to 1; default: 1).
group_neg_corr	Whether to group negatively correlated features together (e.g. c(0,1) and c(1,0)).

Value

Dataframe of correlated features where the columns are feature1, feature2, and the correlation between those two features (anything exceeding corr_thresh).

Author(s)

Begüm Topçuoğlu, <topcuoglu.begum@gmail.com>

Zena Lapp, <zenalapp@umich.edu>

Examples

```
set.seed(0)
mat <- matrix(runif(100), nrow = 20)
rownames(mat) <- 1:nrow(mat)
colnames(mat) <- 1:ncol(mat)
get_corr_feats(mat, 0.4)
```

 get_feature_importance

Get feature importance using permutation method

Description

Calculates feature importance using a trained model and test data. Requires the `future.apply` package.

Usage

```
get_feature_importance(
  trained_model,
  train_data,
  test_data,
  outcome_colname,
  perf_metric_function,
  perf_metric_name,
  class_probs,
  method,
  seed = NA,
  corr_thresh = 1
)
```

Arguments

<code>trained_model</code>	Trained model from <code>caret::train()</code> .
<code>train_data</code>	Training data: dataframe of outcome and features.
<code>test_data</code>	Held out test data: dataframe of outcome and features.
<code>outcome_colname</code>	Column name as a string of the outcome variable (default NULL; the first column will be chosen automatically).
<code>perf_metric_function</code>	Function to calculate the performance metric to be used for cross-validation and test performance. Some functions are provided by caret (see <code>caret::defaultSummary()</code>). Defaults: binary classification = <code>twoClassSummary</code> , multi-class classification = <code>multiClassSummary</code> , regression = <code>defaultSummary</code> .
<code>perf_metric_name</code>	The column name from the output of the function provided to <code>perf_metric_function</code> that is to be used as the performance metric. Defaults: binary classification = "ROC", multi-class classification = "logLoss", regression = "RMSE".
<code>class_probs</code>	Whether to use class probabilities (TRUE for categorical outcomes, FALSE for numeric outcomes).
<code>method</code>	ML method. Options: <code>c("glmnet", "rf", "rpart2", "svmRadial", "xgbTree")</code> . <ul style="list-style-type: none"> • <code>glmnet</code>: linear, logistic, or multiclass regression

	<ul style="list-style-type: none"> • rf: random forest • rpart2: decision tree • svmRadial: support vector machine • xgbTree: xgboost
seed	Random seed (default: NA). Your results will only be reproducible if you set a seed.
corr_thresh	For feature importance, group correlations above or equal to corr_thresh (range 0 to 1; default: 1).

Value

Dataframe with performance metrics for when each feature (or group of correlated features; names) is permuted (perf_metric), and differences between test performance metric and permuted performance metric (perf_metric_diff). The performance metric name (perf_metric_name) and seed (seed) are also returned.

Author(s)

Begüm Topçuoğlu, <topcuoglu.begum@gmail.com>

Zena Lapp, <zenalapp@umich.edu>

Examples

```
results <- run_ml(otu_small, "glmnet", kfold = 2, cv_times = 2)
names(results$trained_model$trainingData)[1] <- "dx"
get_feature_importance(results$trained_model,
  results$trained_model$trainingData, results$test_data,
  "dx",
  multiClassSummary, "AUC",
  class_probs = TRUE, method = "glmnet"
)
```

get_hp_performance *Get hyperparameter performance metrics*

Description

Get hyperparameter performance metrics

Usage

```
get_hp_performance(trained_model)
```

Arguments

trained_model trained model (e.g. from run_ml())

Value

Named list:

- dat: Dataframe of performance metric for each group of hyperparameters.
- params: Hyperparameters tuned.
- metric: Performance metric used.

Author(s)

Zena Lapp, <zenalapp@umich.edu>

Kelly Sovacool <sovacool@umich.edu>

Examples

```
get_hp_performance(otu_mini_bin_results_glmnet$trained_model)
```

get_hyperparams_list *Set hyperparameters based on ML method and dataset characteristics*

Description

For more details see the vignette on [hyperparameter tuning](#).

Usage

```
get_hyperparams_list(dataset, method)
```

Arguments

dataset	Dataframe with an outcome variable and other columns as features.
method	ML method. Options: c("glmnet", "rf", "rpart2", "svmRadial", "xgbTree"). <ul style="list-style-type: none"> • glmnet: linear, logistic, or multiclass regression • rf: random forest • rpart2: decision tree • svmRadial: support vector machine • xgbTree: xgboost

Value

Named list of hyperparameters.

Author(s)

Kelly Sovacool, <sovacool@umich.edu>

Examples

```
get_hyperparams_list(otu_mini_bin, "rf")
get_hyperparams_list(otu_small, "rf")
get_hyperparams_list(otu_mini_bin, "rpart2")
get_hyperparams_list(otu_small, "rpart2")
```

get_outcome_type *Get outcome type.*

Description

If the outcome is numeric, the type is continuous. Otherwise, the outcome type is binary if there are only two outcomes or multiclass if there are more than two outcomes.

Usage

```
get_outcome_type(outcomes_vec)
```

Arguments

outcomes_vec Vector of outcomes.

Value

Outcome type (continuous, binary, or multiclass).

Author(s)

Zena Lapp, <zenalapp@umich.edu>

Examples

```
get_outcome_type(c(1, 2, 1))
get_outcome_type(c("a", "b", "b"))
get_outcome_type(c("a", "b", "c"))
```

get_partition_indices *Select indices to partition the data into training & testing sets.*

Description

Use this function to get the row indices for the training set.

Usage

```
get_partition_indices(outcomes, training_frac = 0.8, groups = NULL)
```

Arguments

outcomes	vector of outcomes
training_frac	max fraction of data for the training set(default: 0.8)
groups	vector of groups. length must match the number of rows in the dataset. (default: NULL)

Details

If groups is NULL, uses [createDataPartition](#). Otherwise, uses `create_grouped_data_partition()`.

Set the seed prior to calling this function if you would like your data partitions to be reproducible (recommended).

Value

Vector of row indices for the training set.

Author(s)

Kelly Sovacool, sovacool@umich.edu

Examples

```
training_inds <- get_partition_indices(otu_mini_bin$dx)
train_data <- otu_mini_bin[training_inds, ]
test_data <- otu_mini_bin[-training_inds, ]
```

get_performance_tbl *Get model performance metrics as a one-row tibble*

Description

Get model performance metrics as a one-row tibble

Usage

```
get_performance_tbl(
  trained_model,
  test_data,
  outcome_colname,
  perf_metric_function,
  perf_metric_name,
  class_probs,
  method,
  seed = NA
)
```

Arguments

trained_model	Trained model from <code>caret::train()</code> .
test_data	Held out test data: dataframe of outcome and features.
outcome_colname	Column name as a string of the outcome variable (default NULL; the first column will be chosen automatically).
perf_metric_function	Function to calculate the performance metric to be used for cross-validation and test performance. Some functions are provided by caret (see <code>caret::defaultSummary()</code>). Defaults: binary classification = <code>twoClassSummary</code> , multi-class classification = <code>multiClassSummary</code> , regression = <code>defaultSummary</code> .
perf_metric_name	The column name from the output of the function provided to <code>perf_metric_function</code> that is to be used as the performance metric. Defaults: binary classification = "ROC", multi-class classification = "logLoss", regression = "RMSE".
class_probs	Whether to use class probabilities (TRUE for categorical outcomes, FALSE for numeric outcomes).
method	ML method. Options: <code>c("glmnet", "rf", "rpart2", "svmRadial", "xgbTree")</code> . <ul style="list-style-type: none"> • <code>glmnet</code>: linear, logistic, or multiclass regression • <code>rf</code>: random forest • <code>rpart2</code>: decision tree • <code>svmRadial</code>: support vector machine • <code>xgbTree</code>: xgboost
seed	Random seed (default: NA). Your results will only be reproducible if you set a seed.

Value

A one-row tibble with columns cv_auroc, column for each of the performance metrics for the test data method, and seed.

Author(s)

Kelly Sovacool, <sovacool@umich.edu>

Zena Lapp, <zenalapp@umich.edu>

Examples

```
results <- run_ml(otu_small, "glmnet", kfold = 2, cv_times = 2)
names(results$trained_model$trainingData)[1] <- "dx"
get_performance_tbl(results$trained_model, results$test_data,
  "dx",
  multiClassSummary, "AUC",
  class_probs = TRUE,
  method = "glmnet"
)
```

get_perf_metric_fn *Get default performance metric function*

Description

Get default performance metric function

Usage

```
get_perf_metric_fn(outcome_type)
```

Arguments

outcome_type Type of outcome (one of: "continuous", "binary", "multiclass").

Value

Performance metric function.

Author(s)

Zena Lapp, <zenalapp@umich.edu>

Examples

```
get_perf_metric_fn("continuous")
get_perf_metric_fn("binary")
get_perf_metric_fn("multiclass")
```

`get_perf_metric_name` *Get default performance metric name*

Description

Get default performance metric name for cross-validation.

Usage

```
get_perf_metric_name(outcome_type)
```

Arguments

`outcome_type` Type of outcome (one of: "continuous","binary","multiclass").

Value

Performance metric name.

Author(s)

Zena Lapp, <zenalapp@umich.edu>

Examples

```
get_perf_metric_name("continuous")
get_perf_metric_name("binary")
get_perf_metric_name("multiclass")
```

`get_tuning_grid` *Generate the tuning grid for tuning hyperparameters*

Description

Generate the tuning grid for tuning hyperparameters

Usage

```
get_tuning_grid(hyperparams_list, method)
```

Arguments

- `hyperparams_list` Named list of lists of hyperparameters.
- `method` ML method. Options: `c("glmnet", "rf", "rpart2", "svmRadial", "xgbTree")`.
- `glmnet`: linear, logistic, or multiclass regression
 - `rf`: random forest
 - `rpart2`: decision tree
 - `svmRadial`: support vector machine
 - `xgbTree`: xgboost

Value

The tuning grid.

Author(s)

Begüm Topçuoğlu, <topcuoglu.begum@gmail.com>

Kelly Sovacool, <sovacool@umich.edu>

Examples

```
ml_method <- "glmnet"
hparams_list <- get_hyperparams_list(otu_small, ml_method)
get_tuning_grid(hparams_list, ml_method)
```

mikropml

mikropml: User-Friendly R Package for Robust Machine Learning Pipelines

Description

`mikropml` implements robust machine learning pipelines using regression, support vector machines, decision trees, random forest, or gradient-boosted trees. The main functions are `preprocess_data()` to process your data prior to running machine learning, and `run_ml()` to run machine learning.

Authors

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See vignettes

- [Introduction](#)
- [Preprocessing data](#)
- [Hyperparameter tuning](#)
- [Parallel processing](#)
- [The mikropml paper](#)

`otu_mini_bin`*Mini OTU abundance dataset*

Description

A dataset containing relative abundances of OTUs for human stool samples with a binary outcome, dx. This is a subset of `otu_small`.

Usage

```
otu_mini_bin
```

Format

A data frame. The dx column is the diagnosis: healthy or cancerous (colorectal). All other columns are OTU relative abundances.

`otu_mini_bin_results_glmnet`*Results from running the pipeline with L2 logistic regression on otu_mini_bin with feature importance and grouping*

Description

Results from running the pipeline with L2 logistic regression on `otu_mini_bin` with feature importance and grouping.

Usage

```
otu_mini_bin_results_glmnet
```

Format

An object of class `list` of length 4.

otu_mini_bin_results_rf

Results from running the pipeline with random forest on otu_mini_bin

Description

Results from running the pipeline with random forest on otu_mini_bin

Usage

```
otu_mini_bin_results_rf
```

Format

An object of class list of length 4.

otu_mini_bin_results_rpart2

Results from running the pipeline with rpart2 on otu_mini_bin

Description

Results from running the pipeline with rpart2 on otu_mini_bin

Usage

```
otu_mini_bin_results_rpart2
```

Format

An object of class list of length 4.

otu_mini_bin_results_svmRadial

Results from running the pipeline with svmRadial on otu_mini_bin

Description

Results from running the pipeline with svmRadial on otu_mini_bin

Usage

```
otu_mini_bin_results_svmRadial
```

Format

An object of class list of length 4.

`otu_mini_bin_results_xgbTree`*Results from running the pipeline with xgbTree on otu_mini_bin*

Description

Results from running the pipeline with xgbTree on otu_mini_bin

Usage`otu_mini_bin_results_xgbTree`**Format**

An object of class list of length 4.

`otu_mini_cont_results_glmnet`*Results from running the pipeline with glmnet on otu_mini_bin with Otu00001 as the outcome*

Description

Results from running the pipeline with glmnet on otu_mini_bin with Otu00001 as the outcome

Usage`otu_mini_cont_results_glmnet`**Format**

An object of class list of length 4.

`otu_mini_cv`*Cross validation on train_data_mini with grouped features.*

Description

Cross validation on train_data_mini with grouped features.

Usage`otu_mini_cv`**Format**

An object of class list of length 27.

otu_mini_multi	<i>Mini OTU abundance dataset with 3 categorical variables</i>
----------------	--

Description

A dataset containing relative abundances of OTUs for human stool samples

Usage

```
otu_mini_multi
```

Format

A data frame The dx column is the colorectal cancer diagnosis: adenoma, carcinoma, normal. All other columns are OTU relative abundances.

otu_mini_multi_results_glmnet	<i>Results from running the pipeline with glmnet on otu_mini_multi for multiclass outcomes</i>
-------------------------------	--

Description

Results from running the pipeline with glmnet on otu_mini_multi for multiclass outcomes

Usage

```
otu_mini_multi_results_glmnet
```

Format

An object of class list of length 4.

otu_small	<i>Small OTU abundance dataset</i>
-----------	------------------------------------

Description

A dataset containing relative abundances of 60 OTUs for 60 human stool samples. This is a subset of the data provided in `extdata/otu_large.csv`, which was used in [Topçuoğlu *et al.* 2020](#).

Usage

```
otu_small
```

Format

A data frame with 60 rows and 61 variables. The `dx` column is the diagnosis: healthy or cancerous (colorectal). All other columns are OTU relative abundances.

plot_hp_performance	<i>Plot hyperparameter performance metrics</i>
---------------------	--

Description

Plot hyperparameter performance metrics

Usage

```
plot_hp_performance(dat, param_col, metric_col)
```

Arguments

<code>dat</code>	dataframe of hyperparameters and performance metric (e.g. from <code>get_hp_performance()</code> or <code>combine_hp_performance()</code>)
<code>param_col</code>	hyperparameter to be plotted. must be a column in <code>dat</code> .
<code>metric_col</code>	performance metric. must be a column in <code>dat</code> .

Value

ggplot of hyperparameter performance.

Author(s)

Zena Lapp, <zenalapp@umich.edu>

Kelly Sovacool <sovacool@umich.edu>

Examples

```
# plot for a single `run_ml()` call
hp_metrics <- get_hp_performance(otu_mini_bin_results_glmnet$strained_model)
hp_metrics
plot_hp_performance(hp_metrics$dat, lambda, AUC)

# plot for multiple `run_ml()` calls
results <- lapply(seq(100, 102), function(seed) {
  run_ml(otu_small, "glmnet", seed = seed)
})
models <- lapply(results, function(x) x$strained_model)
hp_metrics <- combine_hp_performance(models)
plot_hp_performance(hp_metrics$dat, lambda, AUC)
```

plot_model_performance

Plot performance metrics for multiple ML runs with different parameters

Description

ggplot2 is required to use this function.

Usage

```
plot_model_performance(performance_df)
```

Arguments

performance_df dataframe of performance results from multiple calls to run_ml()

Value

A ggplot2 plot of performance.

Author(s)

Begüm Topçuoglu, <topcuoglu.begum@gmail.com>

Kelly Sovacool, <sovacool@umich.edu>

Examples

```
# call `run_ml()` multiple times with different seeds
results_lst <- lapply(seq(100, 104), function(seed) {
  run_ml(otu_small, "glmnet", seed = seed)
})
# extract and combine the performance results
```

```

perf_df <- lapply(results_lst, function(result) {
  result[["performance"]]
}) %>%
  dplyr::bind_rows()
# plot the performance results
p <- plot_model_performance(perf_df)

# call `run_ml()` with different ML methods
param_grid <- expand_grid(
  seeds = seq(100, 104),
  methods = c("glmnet", "rf")
)
results_mtx <- mapply(
  function(seed, method) {
    run_ml(otu_mini_bin, method, seed = seed, kfold = 2)
  },
  param_grid$seeds, param_grid$methods
)
# extract and combine the performance results
perf_df2 <- dplyr::bind_rows(results_mtx["performance", ])
# plot the performance results
p <- plot_model_performance(perf_df2)

# you can continue adding layers to customize the plot
p +
  theme_classic() +
  scale_color_brewer(palette = "Dark2") +
  coord_flip()

```

preprocess_data

Preprocess data prior to running machine learning

Description

Function to preprocess your data for input into [run_ml\(\)](#).

Usage

```

preprocess_data(
  dataset,
  outcome_colname,
  method = c("center", "scale"),
  remove_var = "nzv",
  collapse_corr_feats = TRUE,
  to_numeric = TRUE,
  group_neg_corr = TRUE
)

```

Arguments

dataset	Dataframe with an outcome variable and other columns as features.
outcome_colname	Column name as a string of the outcome variable (default NULL; the first column will be chosen automatically).
method	Methods to preprocess the data, described in <code>caret::preProcess()</code> (default: <code>c("center", "scale")</code>), use NULL for no normalization).
remove_var	Whether to remove variables with near-zero variance (<code>'nzv'</code> ; default), zero variance (<code>'zv'</code>), or none (NULL).
collapse_corr_feats	Whether to keep only one of perfectly correlated features.
to_numeric	Whether to change features to numeric where possible.
group_neg_corr	Whether to group negatively correlated features together (e.g. <code>c(0,1)</code> and <code>c(1,0)</code>).

Value

Named list including:

- `dat_transformed`: Preprocessed data.
- `grp_feats`: If features were grouped together, a named list of the features corresponding to each group.
- `removed_feats`: Any features that were removed during preprocessing (e.g. because there was zero variance or near-zero variance for those features).

More details

See the [preprocessing vignette](#) for more details.

Author(s)

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Examples

```
preprocess_data(mikropml::otu_small, "dx")
```

```
randomize_feature_order
```

Randomize feature order to eliminate any position-dependent effects

Description

Randomize feature order to eliminate any position-dependent effects

Usage

```
randomize_feature_order(dataset, outcome_colname)
```

Arguments

`dataset` Dataframe with an outcome variable and other columns as features.
`outcome_colname` Column name as a string of the outcome variable (default NULL; the first column will be chosen automatically).

Value

Dataset with feature order randomized.

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Examples

```
dat <- data.frame(  
  outcome = c("1", "2", "3"),  
  a = 4:6, b = 7:9, c = 10:12, d = 13:15  
)  
randomize_feature_order(dat, "outcome")
```

run_ml

Run the machine learning pipeline

Description

This function runs machine learning (ML), evaluates the best model, and optionally calculates feature importance using a robust framework outlined in Topçuoğlu *et al.* 2020 ([doi:10.1128/mBio.00434-20](https://doi.org/10.1128/mBio.00434-20)). Required inputs are a dataframe with an outcome variable and other columns as features, as well as the ML method. See `vignette('introduction')` for more details.

Usage

```
run_ml(  
  dataset,  
  method,  
  outcome_colname = NULL,  
  hyperparameters = NULL,  
  find_feature_importance = FALSE,  
  kfold = 5,  
  cv_times = 100,
```

```

training_frac = 0.8,
perf_metric_function = NULL,
perf_metric_name = NULL,
groups = NULL,
corr_thresh = 1,
ntree = 1000,
seed = NA
)

```

Arguments

dataset	Dataframe with an outcome variable and other columns as features.
method	ML method. Options: <code>c("glmnet", "rf", "rpart2", "svmRadial", "xgbTree")</code> . <ul style="list-style-type: none"> • <code>glmnet</code>: linear, logistic, or multiclass regression • <code>rf</code>: random forest • <code>rpart2</code>: decision tree • <code>svmRadial</code>: support vector machine • <code>xgbTree</code>: xgboost
outcome_colname	Column name as a string of the outcome variable (default <code>NULL</code> ; the first column will be chosen automatically).
hyperparameters	Dataframe of hyperparameters (default <code>NULL</code> ; sensible defaults will be chosen automatically).
find_feature_importance	Run permutation importance (default: <code>FALSE</code>). <code>TRUE</code> is recommended if you would like to identify features important for predicting your outcome, but it is resource-intensive.
kfold	Fold number for k-fold cross-validation (default: 5).
cv_times	Number of cross-validation partitions to create (default: 100).
training_frac	Fraction of data for training set (default: 0.8). The remaining data will be used in the testing set.
perf_metric_function	Function to calculate the performance metric to be used for cross-validation and test performance. Some functions are provided by <code>caret</code> (see <code>caret::defaultSummary()</code>). Defaults: binary classification = <code>twoClassSummary</code> , multi-class classification = <code>multiClassSummary</code> , regression = <code>defaultSummary</code> .
perf_metric_name	The column name from the output of the function provided to <code>perf_metric_function</code> that is to be used as the performance metric. Defaults: binary classification = <code>"ROC"</code> , multi-class classification = <code>"logLoss"</code> , regression = <code>"RMSE"</code> .
groups	Vector of groups to keep together when splitting the data into train and test sets, and for cross-validation. length matches the number of rows in the dataset (default: <code>NULL</code>).

corr_thresh	For feature importance, group correlations above or equal to corr_thresh (range 0 to 1; default: 1).
ntree	For random forest, how many trees to use (default: 1000). Note that caret doesn't allow this parameter to be tuned.
seed	Random seed (default: NA). Your results will only be reproducible if you set a seed.

Value

Named list with results:

- `trained_model`: Output of `caret::train()`, including the best model.
- `test_data`: Part of the data that was used for testing.
- `performance`: Dataframe of performance metrics. The first column is the cross-validation performance metric, and the last two columns are the ML method used and the seed (if one was set), respectively. All other columns are performance metrics calculated on the test data. This contains only one row, so you can easily combine performance dataframes from multiple calls to `run_ml()` (see `vignette("parallel")`).
- `feature_importance`: If feature importances were calculated, a dataframe where each row is a feature or correlated group. The columns are the performance metric of the permuted data, the difference between the true performance metric and the performance metric of the permuted data (true - permuted), the feature name, the ML method, the performance metric name, and the seed (if provided). For AUC and RMSE, the higher `perf_metric_diff` is, the more important that feature is for predicting the outcome. For log loss, the lower `perf_metric_diff` is, the more important that feature is for predicting the outcome.

More details

For more details, please see [the vignettes](#).

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Examples

```
run_ml(otu_small, "glmnet",
  seed = 2019
)
run_ml(otu_small, "rf",
  outcome_colname = "dx",
  find_feature_importance = TRUE
)
```

tidy_perf_data	<i>Tidy the performance dataframe</i>
----------------	---------------------------------------

Description

Used by `plot_model_performance()`.

Usage

```
tidy_perf_data(performance_df)
```

Arguments

`performance_df` dataframe of performance results from multiple calls to `run_ml()`

Value

Tidy dataframe with model performance metrics.

Author(s)

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Examples

```
# call `run_ml()` multiple times with different seeds
results_lst <- lapply(seq(100, 104), function(seed) {
  run_ml(otu_small, "glmnet", seed = seed)
})
# extract and combine the performance results
perf_df <- lapply(results_lst, function(result) {
  result[["performance"]]
}) %>%
  dplyr::bind_rows()
# make it pretty!
tidy_perf_data(perf_df)
```

train_model	<i>Train model</i>
-------------	--------------------

Description

Train model using `caret::train()`.

Usage

```
train_model(
  model_formula,
  train_data,
  method,
  cv,
  perf_metric_name,
  tune_grid,
  ntree
)
```

Arguments

model_formula	Model formula.
train_data	Training data.
method	ML method. Options: <code>c("glmnet", "rf", "rpart2", "svmRadial", "xgbTree")</code> . <ul style="list-style-type: none"> • <code>glmnet</code>: linear, logistic, or multiclass regression • <code>rf</code>: random forest • <code>rpart2</code>: decision tree • <code>svmRadial</code>: support vector machine • <code>xgbTree</code>: xgboost
cv	Cross-validation caret scheme.
perf_metric_name	The column name from the output of the function provided to <code>perf_metric_function</code> that is to be used as the performance metric. Defaults: binary classification = "ROC", multi-class classification = "logLoss", regression = "RMSE".
tune_grid	Tuning grid.
ntree	For random forest, how many trees to use (default: 1000). Note that caret doesn't allow this parameter to be tuned.

Details

TODO: Add example.

Value

Trained model from `caret::train()`.

Author(s)

Zena Lapp, <zenalapp@umich.edu>

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