

Package ‘mikropml’

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Title User-Friendly R Package for Supervised Machine Learning Pipelines

Version 1.7.0

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](https://doi.org/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 <<https://www.schlosslab.org/mikropml/>> for more information, documentation, and examples.

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

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

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bootstrap_performance Calculate a bootstrap confidence interval for the performance on a single train/test split

Description

Uses `rsample::bootstraps()`, `rsample::int_pctl()`, and `furrr::future_map()`

Usage

```
bootstrap_performance(  
  ml_result,  
  outcome_colname,  
  bootstrap_times = 10000,  
  alpha = 0.05  
)
```

Arguments

<code>ml_result</code>	result returned from a single <code>run_ml()</code> call
<code>outcome_colname</code>	Column name as a string of the outcome variable (default NULL; the first column will be chosen automatically).
<code>bootstrap_times</code>	the number of bootstraps to create (default: 10000)
<code>alpha</code>	the alpha level for the confidence interval (default 0.05 to create a 95% confidence interval)

Value

a data frame with an estimate (.estimate), lower bound (.lower), and upper bound (.upper) for each performance metric (term).

Author(s)

Kelly Sovacool, <sovacool@umich.edu>

Examples

```
bootstrap_performance(otu_mini_bin_results_glmnet, "dx",
  bootstrap_times = 10, alpha = 0.10
)
## Not run:
outcome_colname <- "dx"
run_ml(otu_mini_bin, "rf", outcome_colname = "dx") %>%
  bootstrap_performance(outcome_colname,
    bootstrap_times = 10000,
    alpha = 0.05
  )

## End(Not run)
```

calc_balanced_precision

Calculate balanced precision given actual and baseline precision

Description

Implements Equation 1 from Wu *et al.* 2021 [doi:10.1016/j.ajhg.2021.08.012](https://doi.org/10.1016/j.ajhg.2021.08.012). It is the same as Equation 7 if AUPRC (aka prAUC) is used in place of precision.

Usage

```
calc_balanced_precision(precision, prior)
```

Arguments

precision actual precision of the model.
prior baseline precision, aka frequency of positives. Can be calculated with [calc_baseline_precision](#)

Value

the expected precision if the data were balanced

Author(s)

Kelly Sovacool <sovacool@umich.edu>

Examples

```

prior <- calc_baseline_precision(otu_mini_bin,
  outcome_colname = "dx",
  pos_outcome = "cancer"
)
calc_balanced_precision(otu_mini_bin_results_rf$performance$Precision, prior)

otu_mini_bin_results_rf$performance %>%
  dplyr::mutate(
    balanced_precision = calc_balanced_precision(Precision, prior),
    aubprc = calc_balanced_precision(prAUC, prior)
  ) %>%
  dplyr::select(AUC, Precision, balanced_precision, aubprc)

# cumulative performance for a single model
sensspec_1 <- calc_model_sensspec(
  otu_mini_bin_results_glmnet$trained_model,
  otu_mini_bin_results_glmnet$test_data,
  "dx"
)
head(sensspec_1)
prior <- calc_baseline_precision(otu_mini_bin,
  outcome_colname = "dx",
  pos_outcome = "cancer"
)
sensspec_1 %>%
  dplyr::mutate(balanced_precision = calc_balanced_precision(precision, prior)) %>%
  dplyr::rename(recall = sensitivity) %>%
  calc_mean_perf(group_var = recall, sum_var = balanced_precision) %>%
  plot_mean_prc(ycol = mean_balanced_precision)

```

calc_baseline_precision

Calculate the fraction of positives, i.e. baseline precision for a PRC curve

Description

Calculate the fraction of positives, i.e. baseline precision for a PRC curve

Usage

```
calc_baseline_precision(dataset, outcome_colname = NULL, pos_outcome = NULL)
```

Arguments

dataset Data frame with an outcome variable and other columns as features. Alternatively, the input can be in TreeSummarizedExperiment format.

outcome_colname Column name as a string of the outcome variable (default NULL; the first column will be chosen automatically).

pos_outcome the positive outcome from outcome_colname, e.g. "cancer" for the otu_mini_bin dataset.

Value

the baseline precision based on the fraction of positives

Author(s)

Kelly Sovacool, <sovacool@umich.edu>

Examples

```
# calculate the baseline precision
data.frame(y = c("a", "b", "a", "b")) %>%
  calc_baseline_precision(
    outcome_colname = "y",
    pos_outcome = "a"
  )

calc_baseline_precision(otu_mini_bin,
  outcome_colname = "dx",
  pos_outcome = "cancer"
)

# if you're not sure which outcome was used as the 'positive' outcome during
# model training, you can access it from the trained model and pass it along:
calc_baseline_precision(otu_mini_bin,
  outcome_colname = "dx",
  pos_outcome = otu_mini_bin_results_glmnet$strained_model$levels[1]
)
```

calc_mean_perf *Generic function to calculate mean performance curves for multiple models*

Description

Used by calc_mean_roc() and calc_mean_prc().

Usage

```
calc_mean_perf(sensspec_dat, group_var = specificity, sum_var = sensitivity)
```

Arguments

sensspec_dat	data frame created by concatenating results of calc_model_sensspec() for multiple models.
group_var	variable to group by (e.g. specificity or recall).
sum_var	variable to summarize (e.g. sensitivity or precision).

Value

data frame with mean & standard deviation of sum_var summarized over group_var

Author(s)

Courtney Armour
Kelly Sovacool

calc_model_sensspec *Calculate and summarize performance for ROC and PRC plots*

Description

Use these functions to calculate cumulative sensitivity, specificity, recall, etc. on single models, concatenate the results together from multiple models, and compute mean ROC and PRC. You can then plot mean ROC and PRC curves to visualize the results. **Note:** These functions assume a binary outcome.

Usage

```
calc_model_sensspec(trained_model, test_data, outcome_colname = NULL)
```

```
calc_mean_roc(sensspec_dat)
```

```
calc_mean_prc(sensspec_dat)
```

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).
sensspec_dat	data frame created by concatenating results of calc_model_sensspec() for multiple models.

Value

data frame with summarized performance

Functions

- `calc_model_sensspec()`: Get sensitivity, specificity, and precision for a model.
- `calc_mean_roc()`: Calculate mean sensitivity over specificity for multiple models
- `calc_mean_prc()`: Calculate mean precision over recall for multiple models

Author(s)

Courtney Armour

Kelly Sovacool, <sovacool@umich.edu>

Examples

```
## Not run:
library(dplyr)
# get cumulative performance for a single model
sensspec_1 <- calc_model_sensspec(
  otu_mini_bin_results_glmnet$trained_model,
  otu_mini_bin_results_glmnet$test_data,
  "dx"
)
head(sensspec_1)

# get performance for multiple models
get_sensspec_seed <- function(seed) {
  ml_result <- run_ml(otu_mini_bin, "glmnet", seed = seed)
  sensspec <- calc_model_sensspec(
    ml_result$trained_model,
    ml_result$test_data,
    "dx"
  ) %>%
    dplyr::mutate(seed = seed)
  return(sensspec)
}
sensspec_dat <- purrr::map_dfr(seq(100, 102), get_sensspec_seed)

# calculate mean sensitivity over specificity
roc_dat <- calc_mean_roc(sensspec_dat)
head(roc_dat)

# calculate mean precision over recall
prc_dat <- calc_mean_prc(sensspec_dat)
head(prc_dat)

# plot ROC & PRC
roc_dat %>% plot_mean_roc()
baseline_prec <- calc_baseline_precision(otu_mini_bin, "dx", "cancer")
prc_dat %>%
  plot_mean_prc(baseline_precision = baseline_prec)

# balanced precision
prior <- calc_baseline_precision(otu_mini_bin,
```

```

  outcome_colname = "dx",
  pos_outcome = "cancer"
)
bprc_dat <- sensspec_dat %>%
  dplyr::mutate(balanced_precision = calc_balanced_precision(precision, prior)) %>%
  dplyr::rename(recall = sensitivity) %>%
  calc_mean_perf(group_var = recall, sum_var = balanced_precision)
bprc_dat %>% plot_mean_prc(ycol = mean_balanced_precision) + ylab("Mean Bal. Precision")

## End(Not run)

```

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

```
## Not run:
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
)

## End(Not run)
```

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

```
## Not run:
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)

## End(Not run)
```

compare_models	<i>Perform permutation tests to compare the performance metric across all pairs of a group variable.</i>
----------------	--

Description

A wrapper for `permutate_p_value()`.

Usage

```
compare_models(merged_data, metric, group_name, nperm = 10000)
```

Arguments

merged_data	the concatenated performance data from <code>run_ml</code>
metric	metric to compare, must be numeric
group_name	column with group variables to compare
nperm	number of permutations, default=10000

Value

a table of p-values for all pairs of group variable

Author(s)

Courtney R Armour, <armourc@umich.edu>

Examples

```
df <- dplyr::tibble(
  model = c("rf", "rf", "glmnet", "glmnet", "svmRadial", "svmRadial"),
  AUC = c(.2, 0.3, 0.8, 0.9, 0.85, 0.95)
)
set.seed(123)
compare_models(df, "AUC", "model", nperm = 10)
```

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,
  group_partitions = NULL
)
```

Arguments

train_data	Dataframe for training model.
outcome_colname	Column name as a string of the outcome variable (default NULL; the first column will be chosen automatically).
hyperparams_list	Named list of lists of hyperparameters.
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 caret::defaultSummary()). Defaults: binary classification = twoClassSummary, multi-class classification = multiClassSummary, regression = defaultSummary.
class_probs	Whether to use class probabilities (TRUE for categorical outcomes, FALSE for numeric outcomes).
kfold	Fold number for k-fold cross-validation (default: 5).
cv_times	Number of cross-validation partitions to create (default: 100).
groups	Vector of groups to keep together when splitting the data into train and test sets. If the number of groups in the training set is larger than kfold, the groups will also be kept together for cross-validation. Length matches the number of rows in the dataset (default: NULL).
group_partitions	Specify how to assign groups to the training and testing partitions (default: NULL). If groups specifies that some samples belong to group "A" and some

belong to group "B", then setting `group_partitions = list(train = c("A", "B"), test = c("B"))` will result in all samples from group "A" being placed in the training set, some samples from "B" also in the training set, and the remaining samples from "B" in the testing set. The partition sizes will be as close to `training_frac` as possible. If the number of groups in the training set is larger than `kfold`, the groups will also be kept together for cross-validation.

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 <code>caret::preProcess()</code> (default: <code>c("center", "scale")</code>), use <code>NULL</code> 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_feature_importance
```

Get feature importance using the permutation method

Description

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

Usage

```
get_feature_importance(  
  trained_model,  
  test_data,  
  outcome_colname,  
  perf_metric_function,  
  perf_metric_name,  
  class_probs,  
  method,  
  seed = NA,  
  corr_thresh = 1,  
  groups = NULL,  
  nperms = 100,  
  corr_method = "spearman"  
)
```

Arguments

<code>trained_model</code>	Trained model from <code>caret::train()</code> .
<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).

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 caret::defaultSummary()). Defaults: binary classification = twoClassSummary, multi-class classification = multiClassSummary, regression = defaultSummary.
perf_metric_name	The column name from the output of the function provided to perf_metric_function 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: 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
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).
groups	Vector of feature names to group together during permutation. Each element should be a string with feature names separated by a pipe character (). If this is NULL (default), correlated features will be grouped together based on corr_thresh.
nperms	number of permutations to perform (default: 100).
corr_method	Correlation method. Options are the same as those supported by stats::cor: spearman, pearson, kendall. (default: spearman)

Details

For permutation tests, the p-value is the number of permutation statistics that are greater than the test statistic, divided by the number of permutations. In our case, the permutation statistic is the model performance (e.g. AUROC) after randomizing the order of observations for one feature, and the test statistic is the actual performance on the test data. By default we perform 100 permutations per feature; increasing this will increase the precision of estimating the null distribution, but also increases runtime. The p-value represents the probability of obtaining the actual performance in the event that the null hypothesis is true, where the null hypothesis is that the feature is not important for model performance.

We strongly recommend providing multiple cores to speed up computation time. See [our vignette on parallel processing](#) for more details.

Value

Data frame with performance metrics for when each feature (or group of correlated features; feat) is permuted (perf_metric), differences between the actual test performance metric on and the

permuted performance metric (`perf_metric_diff`; test minus permuted performance), and the p-value (pvalue: the probability of obtaining the actual performance value under the null hypothesis). Features with a larger `perf_metric_diff` are more important. 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>

Kelly Sovacool, <sovacool@umich.edu>

Examples

```
## Not run:
# If you called `run_ml()` with `feature_importance = FALSE` (the default),
# you can use `get_feature_importance()` later as long as you have the
# trained model and test data.
results <- run_ml(otu_small, "glmnet", kfold = 2, cv_times = 2)
names(results$trained_model$trainingData)[1] <- "dx"
feat_imp <- get_feature_importance(results$trained_model,
  results$trained_model$trainingData,
  results$test_data,
  "dx",
  multiClassSummary,
  "AUC",
  class_probs = TRUE,
  method = "glmnet"
)

# We strongly recommend providing multiple cores to speed up computation time.
# Do this before calling `get_feature_importance()`.
doFuture::registerDoFuture()
future::plan(future::multicore, workers = 2)

# Optionally, you can group features together with a custom grouping
feat_imp <- get_feature_importance(results$trained_model,
  results$trained_model$trainingData,
  results$test_data,
  "dx",
  multiClassSummary,
  "AUC",
  class_probs = TRUE,
  method = "glmnet",
  groups = c(
    "Otu00007", "Otu00008", "Otu00009", "Otu00011", "Otu00012",
    "Otu00015", "Otu00016", "Otu00018", "Otu00019", "Otu00020", "Otu00022",
    "Otu00023", "Otu00025", "Otu00028", "Otu00029", "Otu00030", "Otu00035",
    "Otu00036", "Otu00037", "Otu00038", "Otu00039", "Otu00040", "Otu00047",
    "Otu00050", "Otu00052", "Otu00054", "Otu00055", "Otu00056", "Otu00060",
    "Otu00003|Otu00002|Otu00005|Otu00024|Otu00032|Otu00041|Otu00053",
    "Otu00014|Otu00021|Otu00017|Otu00031|Otu00057",
    "Otu00013|Otu00006", "Otu00026|Otu00001|Otu00034|Otu00048",
```

```

      "Otu00033|Otu00010",
      "Otu00042|Otu00004", "Otu00043|Otu00027|Otu00049", "Otu00051|Otu00045",
      "Otu00058|Otu00044", "Otu00059|Otu00046"
    )
  )

# the function can show a progress bar if you have the `progressr` package installed.
## optionally, specify the progress bar format:
progressr::handlers(progressr::handler_progress(
  format = ":message :bar :percent | elapsed: :elapsed | eta: :eta",
  clear = FALSE,
  show_after = 0
))
## tell progressr to always report progress
progressr::handlers(global = TRUE)
## run the function and watch the live progress updates
feat_imp <- get_feature_importance(results$trained_model,
  results$trained_model$trainingData,
  results$test_data,
  "dx",
  multiClassSummary,
  "AUC",
  class_probs = TRUE,
  method = "glmnet"
)

# You can specify any correlation method supported by `stats::cor`:
feat_imp <- get_feature_importance(results$trained_model,
  results$trained_model$trainingData,
  results$test_data,
  "dx",
  multiClassSummary,
  "AUC",
  class_probs = TRUE,
  method = "glmnet",
  corr_method = "pearson"
)

## End(Not run)

```

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	Data frame with an outcome variable and other columns as features. Alternatively, the input can be in TreeSummarizedExperiment format.
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,  
  group_partitions = NULL  
)
```

Arguments

outcomes	vector of outcomes
training_frac	Fraction of data for training set (default: 0.8). Rows from the dataset will be randomly selected for the training set, and all remaining rows will be used in the testing set. Alternatively, if you provide a vector of integers, these will be used as the row indices for the training set. All remaining rows will be used in the testing set.
groups	Vector of groups to keep together when splitting the data into train and test sets. If the number of groups in the training set is larger than kfold, the groups will also be kept together for cross-validation. Length matches the number of rows in the dataset (default: NULL).
group_partitions	Specify how to assign groups to the training and testing partitions (default: NULL). If groups specifies that some samples belong to group "A" and some belong to group "B", then setting group_partitions = list(train = c("A", "B"), test = c("B")) will result in all samples from group "A" being placed in the training set, some samples from "B" also in the training set, and the remaining samples from "B" in the testing set. The partition sizes will be as close to training_frac as possible. If the number of groups in the training set is larger than kfold, the groups will also be kept together for cross-validation.

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 `caret::train()`.

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 `caret::defaultSummary()`). Defaults: binary classification = `twoClassSummary`, multi-class classification = `multiClassSummary`, regression = `defaultSummary`.

perf_metric_name The column name from the output of the function provided to `perf_metric_function` 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: 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
seed	Random seed (default: NA). Your results will only be reproducible if you set a seed.

Value

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

Author(s)

Kelly Sovacool, <sovacool@umich.edu>

Zena Lapp, <zenalapp@umich.edu>

Examples

```
## Not run:
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"
)

## End(Not run)
```

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	<i>Generate the tuning grid for tuning hyperparameters</i>
-----------------	--

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)
```

group_correlated_features
Group correlated features

Description

Group correlated features

Usage

```
group_correlated_features(  
  features,  
  corr_thresh = 1,  
  group_neg_corr = TRUE,  
  corr_method = "spearman"  
)
```

Arguments

features a dataframe with each column as a feature for ML

corr_thresh 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)`).

corr_method Correlation method. Options are the same as those supported by `stats::cor`: `spearman`, `pearson`, `kendall`. (default: `spearman`)

Value

vector where each element is a group of correlated features separated by pipes (`|`)

Author(s)

Kelly Sovacool, <sovacool@umich.edu>

Examples

```
features <- data.frame(  
  a = 1:3, b = 2:4, c = c(1, 0, 1),  
  d = (5:7), e = c(5, 1, 4), f = c(-1, 0, -1)  
)  
group_correlated_features(features)
```

otu_data_preproc	<i>Mini OTU abundance dataset - preprocessed</i>
------------------	--

Description

This is the result of running `preprocess_data("otu_mini_bin")`

Usage

```
otu_data_preproc
```

Format

An object of class `list` of length 3.

otu_mini_bin	<i>Mini OTU abundance dataset</i>
--------------	-----------------------------------

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	<i>Results from running the pipeline with L2 logistic regression on otu_mini_bin with feature importance and grouping</i>
-----------------------------	---

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_cont_results_nocv

Results from running the pipeline with glmnet on otu_mini_bin with Otu00001 as the outcome column, using a custom train control scheme that does not perform cross-validation

Description

Results from running the pipeline with glmnet on otu_mini_bin with Otu00001 as the outcome column, using a custom train control scheme that does not perform cross-validation

Usage

otu_mini_cont_results_nocv

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 *Mini OTU abundance dataset with 3 categorical variables*

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_group *Groups for otu_mini_multi*

Description

Groups for otu_mini_multi

Usage

otu_mini_multi_group

Format

An object of class character of length 490.

`otu_mini_multi_results_glmnet`

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

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`

Small OTU abundance dataset

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.

permute_p_value	<i>Calculated a permuted p-value comparing two models</i>
-----------------	---

Description

Calculated a permuted p-value comparing two models

Usage

```
permute_p_value(  
  merged_data,  
  metric,  
  group_name,  
  group_1,  
  group_2,  
  nperm = 10000  
)
```

Arguments

merged_data	the concatenated performance data from run_ml
metric	metric to compare, must be numeric
group_name	column with group variables to compare
group_1	name of one group to compare
group_2	name of other group to compare
nperm	number of permutations, default=10000

Value

numeric p-value comparing two models

Author(s)

Begüm Topçuoğlu, <topcuoglu.begum@gmail.com>
Courtney R Armour, <armourc@umich.edu>

Examples

```
df <- dplyr::tibble(  
  model = c("rf", "rf", "glmnet", "glmnet", "svmRadial", "svmRadial"),  
  AUC = c(.2, 0.3, 0.8, 0.9, 0.85, 0.95)  
)  
set.seed(123)  
permute_p_value(df, "AUC", "model", "rf", "glmnet", nperm = 100)
```

plot_hp_performance *Plot hyperparameter performance metrics*

Description

Plot hyperparameter performance metrics

Usage

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

Arguments

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

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$trained_model)
hp_metrics
plot_hp_performance(hp_metrics$dat, lambda, AUC)
## Not run:
# 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$trained_model)
hp_metrics <- combine_hp_performance(models)
plot_hp_performance(hp_metrics$dat, lambda, AUC)

## End(Not run)
```

plot_mean_roc

*Plot ROC and PRC curves***Description**

Plot ROC and PRC curves

Usage

```
plot_mean_roc(dat, ribbon_fill = "#C6DBEF", line_color = "#08306B")

plot_mean_prc(
  dat,
  baseline_precision = NULL,
  ycol = mean_precision,
  ribbon_fill = "#C7E9C0",
  line_color = "#00441B"
)
```

Arguments

dat	sensitivity, specificity, and precision data calculated by calc_mean_roc()
ribbon_fill	ribbon fill color (default: "#D9D9D9")
line_color	line color (default: "#000000")
baseline_precision	baseline precision from calc_baseline_precision()
ycol	column for the y axis (Default: mean_precision)

Functions

- plot_mean_roc(): Plot mean sensitivity over specificity
- plot_mean_prc(): Plot mean precision over recall

Author(s)

Courtney Armour
 Kelly Sovacool <sovacool@umich.edu>

Examples

```
## Not run:
library(dplyr)
# get performance for multiple models
get_sensspec_seed <- function(seed) {
  ml_result <- run_ml(otu_mini_bin, "glmnet", seed = seed)
  sensspec <- calc_model_sensspec(
```

```
      ml_result$trained_model,
      ml_result$test_data,
      "dx"
    ) %>%
      mutate(seed = seed)
    return(sensspec)
  }
sensspec_dat <- purrr::map_dfr(seq(100, 102), get_sensspec_seed)

# plot ROC & PRC
sensspec_dat %>%
  calc_mean_roc() %>%
  plot_mean_roc()
baseline_prec <- calc_baseline_precision(otu_mini_bin, "dx", "cancer")
sensspec_dat %>%
  calc_mean_prc() %>%
  plot_mean_prc(baseline_precision = baseline_prec)

## End(Not run)
```

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

```

## Not run:
# 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()

## End(Not run)

```

preprocess_data

Preprocess data prior to running machine learning

Description

Function to preprocess your data for input into `run_ml()`.

Usage

```
preprocess_data(dataset, ...)
```

```

## S4 method for signature 'TreeSummarizedExperiment'
preprocess_data(
  dataset,
  outcome_colname,
  assay.type = "counts",
  col.var = NULL,
  altexp = NULL,
  name = "preprocessed",
  ...
)

## S4 method for signature 'ANY'
preprocess_data(
  dataset,
  outcome_colname,
  method = c("center", "scale"),
  remove_var = "nzv",
  collapse_corr_feats = TRUE,
  corr_method = "spearman",
  corr_thresh = 1,
  to_numeric = TRUE,
  group_neg_corr = TRUE,
  prefilter_threshold = 1,
  ...
)

```

Arguments

dataset	Data frame with an outcome variable and other columns as features. Alternatively, the input can be in <code>TreeSummarizedExperiment</code> format.
...	All additional arguments are passed on to <code>caret::train()</code> , such as case weights via the <code>weights</code> argument or <code>ntree</code> for <code>rf</code> models. See the <code>caret::train()</code> docs for more details.
outcome_colname	Column name as a string of the outcome variable (default <code>NULL</code> ; the first column will be chosen automatically).
assay.type	The name of assay from dataset when the object is in <code>TreeSummarizedExperiment</code> format. This assay is used as an input.
col.var	The name of sample matdata variables from <code>colData</code> slot of dataset when the object is in <code>TreeSummarizedExperiment</code> format. These variables are used as predictors.
altexp	The name of alternative experiment (<code>altExp</code>) from dataset when the object is in <code>TreeSummarizedExperiment</code> format. This can be used to select an experiment for the input.
name	Name of results used when the input is <code>TreeSummarizedExperiment</code> . This same name is used for assay and <code>altExp</code> .

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 correlated features (see <code>corr_method</code> and <code>corr_thresh</code>)
corr_method	Correlation method. Options are the same as those supported by <code>stats::cor</code> : <code>spearman</code> , <code>pearson</code> , <code>kendall</code> . (default: <code>spearman</code>)
corr_thresh	group correlations above or equal to <code>corr_thresh</code> (range 0 to 1; default: 1).
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>).
prefilter_threshold	Remove features which only have non-zero & non-NA values in N rows or fewer (default: 1). Set this to -1 to keep all columns at this step. This step will also be skipped if <code>to_numeric</code> is set to FALSE.

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).

If the input is `TreeSummarizedExperiment`, the output is added as an additional data to the input object. If the set of features match in output and input, the results are stored directly to `assay` slot. If they do not match, the output is stored to `altExp` slot of the object.

If the `progressr` package is installed, a progress bar with time elapsed and estimated time to completion can be displayed.

More details

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

Note that if any values in `outcome_colname` contain spaces, they will be converted to underscores for compatibility with `caret`.

Author(s)

Zena Lapp, <zenalapp@umich.edu>

Kelly Sovacool, <sovacool@umich.edu>

Examples

```

preprocess_data(mikropml::otu_small, "dx")

# the function can show a progress bar if you have the progressr package installed
## optionally, specify the progress bar format
progressr::handlers(progressr::handler_progress(
  format = ":message :bar :percent | elapsed: :elapsed | eta: :eta",
  clear = FALSE,
  show_after = 0
))
## tell progressor to always report progress
## Not run:
progressr::handlers(global = TRUE)
## run the function and watch the live progress updates
dat_preproc <- preprocess_data(mikropml::otu_small, "dx")

# Create TreeSE object
library(TreeSummarizedExperiment)
df <- mikropml::otu_small
assay <- df[, !colnames(df) %in% c("dx"), drop = FALSE] |> t() |> as.matrix()
tse <- TreeSummarizedExperiment(assays = SimpleList(counts = assay))
colData(tse)[["dx"]] <- df[["dx"]]

# Preprocess
tse <- preprocess_data(
  dataset = tse,
  assay.type = "counts",
  outcome_colname = "dx"
)
# The result is in assay slot
tse

## End(Not run)

```

```
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` Data frame with an outcome variable and other columns as features. Alternatively, the input can be in `TreeSummarizedExperiment` format.

`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.

Author(s)

Nick Lesniak, <nlesniak@umich.edu>
 Kelly Sovacool, <sovacool@umich.edu>

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")
```

`remove_singleton_columns`

Remove columns appearing in only threshold row(s) or fewer.

Description

Removes columns which only have non-zero & non-NA values in threshold row(s) or fewer.

Usage

```
remove_singleton_columns(dat, threshold = 1)
```

Arguments

`dat` dataframe

`threshold` Number of rows. If a column only has non-zero & non-NA values in threshold row(s) or fewer, it will be removed.

Value

dataframe without singleton columns

Author(s)

Kelly Sovacool, <sovacool@umich.edu>

Courtney Armour

Examples

```
remove_singleton_columns(data.frame(a = 1:3, b = c(0, 1, 0), c = 4:6))
remove_singleton_columns(data.frame(a = 1:3, b = c(0, 1, 0), c = 4:6), threshold = 0)
remove_singleton_columns(data.frame(a = 1:3, b = c(0, 1, NA), c = 4:6))
remove_singleton_columns(data.frame(a = 1:3, b = c(1, 1, 1), c = 4:6))
```

replace_spaces	<i>Replace spaces in all elements of a character vector with underscores</i>
----------------	--

Description

Replace spaces in all elements of a character vector with underscores

Usage

```
replace_spaces(x, new_char = "_")
```

Arguments

x	a character vector
new_char	the character to replace spaces (default: _)

Value

character vector with all spaces replaced with new_char

Author(s)

Kelly Sovacool, <sovacool@umich.edu>

Examples

```
dat <- data.frame(
  dx = c("outcome 1", "outcome 2", "outcome 1"),
  a = 1:3, b = c(5, 7, 1)
)
dat$dx <- replace_spaces(dat$dx)
dat
```

`run_ml`*Run the machine learning pipeline*

Description

This function splits the data set into a train & test set, trains machine learning (ML) models using k-fold cross-validation, evaluates the best model on the held-out test set, and optionally calculates feature importance using the framework outlined in Topçuoğlu *et al.* 2020 ([doi:10.1128/mBio.0043420](https://doi.org/10.1128/mBio.0043420)). Required inputs are a data frame (must contain an outcome variable and all other columns as features) and the ML method. See `vignette('introduction')` for more details.

Usage

```
run_ml(dataset, ...)

## S4 method for signature 'TreeSummarizedExperiment'
run_ml(
  dataset,
  method,
  outcome_colname,
  assay.type = "counts",
  col.var = NULL,
  altexp = NULL,
  ...
)

## S4 method for signature 'ANY'
run_ml(
  dataset,
  method,
  outcome_colname = NULL,
  hyperparameters = NULL,
  find_feature_importance = FALSE,
  calculate_performance = TRUE,
  kfold = 5,
  cv_times = 100,
  cross_val = NULL,
  training_frac = 0.8,
  perf_metric_function = NULL,
  perf_metric_name = NULL,
  groups = NULL,
  group_partitions = NULL,
  corr_thresh = 1,
  seed = NA,
  ...
)
```

Arguments

dataset	Data frame with an outcome variable and other columns as features. Alternatively, the input can be in <code>TreeSummarizedExperiment</code> format.
...	All additional arguments are passed on to <code>caret::train()</code> , such as case weights via the <code>weights</code> argument or <code>ntree</code> for <code>rf</code> models. See the <code>caret::train()</code> docs for more details.
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).
assay.type	The name of assay from dataset when the object is in <code>TreeSummarizedExperiment</code> format. This assay is used as an input.
col.var	The name of sample matdata variables from <code>colData</code> slot of dataset when the object is in <code>TreeSummarizedExperiment</code> format. These variables are used as predictors.
altexp	The name of alternative experiment (<code>altExp</code>) from dataset when the object is in <code>TreeSummarizedExperiment</code> format. This can be used to select an experiment for the input.
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.
calculate_performance	Whether to calculate performance metrics (default: <code>TRUE</code>). You might choose to skip this if you do not perform cross-validation during model training.
kfold	Fold number for k-fold cross-validation (default: 5).
cv_times	Number of cross-validation partitions to create (default: 100).
cross_val	a custom cross-validation scheme from <code>caret::trainControl()</code> (default: <code>NULL</code> , uses <code>kfold</code> cross validation repeated <code>cv_times</code>). <code>kfold</code> and <code>cv_times</code> are ignored if the user provides a custom cross-validation scheme. See the <code>caret::trainControl()</code> docs for information on how to use it.
training_frac	Fraction of data for training set (default: 0.8). Rows from the dataset will be randomly selected for the training set, and all remaining rows will be used in the testing set. Alternatively, if you provide a vector of integers, these will be used as the row indices for the training set. All remaining rows 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 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".
groups	Vector of groups to keep together when splitting the data into train and test sets. If the number of groups in the training set is larger than <code>kfold</code> , the groups will also be kept together for cross-validation. Length matches the number of rows in the dataset (default: NULL).
group_partitions	Specify how to assign groups to the training and testing partitions (default: NULL). If <code>groups</code> specifies that some samples belong to group "A" and some belong to group "B", then setting <code>group_partitions = list(train = c("A", "B"), test = c("B"))</code> will result in all samples from group "A" being placed in the training set, some samples from "B" also in the training set, and the remaining samples from "B" in the testing set. The partition sizes will be as close to <code>training_frac</code> as possible. If the number of groups in the training set is larger than <code>kfold</code> , the groups will also be kept together for cross-validation.
corr_thresh	For feature importance, group correlations above or equal to <code>corr_thresh</code> (range 0 to 1; default: 1).
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`: Data frame 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 data frames from multiple calls to `run_ml()` (see `vignette("parallel")`).
- `feature_importance`: If feature importances were calculated, a data frame 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

```
## Not run:

# regression
run_ml(otu_small, "glmnet",
      seed = 2019
)

# random forest w/ feature importance
run_ml(otu_small, "rf",
      outcome_colname = "dx",
      find_feature_importance = TRUE
)

# custom cross validation & hyperparameters
run_ml(otu_mini_bin[, 2:11],
      "glmnet",
      outcome_colname = "Otu00001",
      seed = 2019,
      hyperparameters = list(lambda = c(1e-04), alpha = 0),
      cross_val = caret::trainControl(method = "none"),
      calculate_performance = FALSE
)

# Create TreeSE dataset
library(TreeSummarizedExperiment)
df <- mikropml::otu_small
assay <- df[, !colnames(df) %in% c("dx"), drop = FALSE] |> t() |> as.matrix()
tse <- TreeSummarizedExperiment(assays = SimpleList(counts = assay))
colData(tse)[["dx"]] <- otu_mini_multi[["dx"]]

# Train model
res <- run_ml(
  tse,
  assay.type = "counts",
  method = "rf",
  outcome_colname = "dx"
)

## End(Not run)
```

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

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Examples

```
## Not run:
# 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)

## End(Not run)
```

train_model	<i>Train model using <code>caret::train()</code>.</i>
-------------	---

Description

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

Usage

```
train_model(
  train_data,
  outcome_colname,
  method,
  cv,
  perf_metric_name,
  tune_grid,
  ...
)
```

Arguments

train_data	Training data. Expected to be a subset of the full dataset.
outcome_colname	Column name as a string of the outcome variable (default NULL; the first column will be chosen automatically).
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 from <code>define_cv()</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".
tune_grid	Tuning grid from <code>get_tuning_grid().#'</code>
...	All additional arguments are passed on to <code>caret::train()</code> , such as case weights via the <code>weights</code> argument or <code>ntree</code> for <code>rf</code> models. See the <code>caret::train()</code> docs for more details.

Value

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

Author(s)

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Examples

```
## Not run:
training_data <- otu_mini_bin_results_glmnet$trained_model$trainingData %>%
  dplyr::rename(dx = .outcome)
method <- "rf"
hyperparameters <- get_hyperparams_list(otu_mini_bin, method)
cross_val <- define_cv(training_data,
  "dx",
  hyperparameters,
  perf_metric_function = caret::multiClassSummary,
  class_probs = TRUE,
  cv_times = 2
)
tune_grid <- get_tuning_grid(hyperparameters, method)

rf_model <- train_model(
  training_data,
  "dx",
  method,
  cross_val,
  "AUC",
  tune_grid,
  ntree = 1000
)
rf_model$results %>% dplyr::select(mtry, AUC, prAUC)

## End(Not run)
```

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