

Package ‘MantaID’

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Title A Machine-Learning Based Tool to Automate the Identification of Biological Database IDs

Version 1.0.4

Description The number of biological databases is growing rapidly, but different databases use different IDs to refer to the same biological entity. The inconsistency in IDs impedes the integration of various types of biological data. To resolve the problem, we developed 'MantaID', a data-driven, machine-learning based approach that automates identifying IDs on a large scale. The 'MantaID' model's prediction accuracy was proven to be 99%, and it correctly and effectively predicted 100,000 ID entries within two minutes. 'MantaID' supports the discovery and exploitation of ID patterns from large quantities of databases. (e.g., up to 542 biological databases). An easy-to-use freely available open-source software R package, a user-friendly web application, and API were also developed for 'MantaID' to improve applicability. To our knowledge, 'MantaID' is the first tool that enables an automatic, quick, accurate, and comprehensive identification of large quantities of IDs, and can therefore be used as a starting point to facilitate the complex assimilation and aggregation of biological data across diverse databases.

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Encoding UTF-8

RoxygenNote 7.3.2

Depends R (>= 4.4.0),biomaRt,caret,keras,mlr3tuning,mlr3

LazyData true

URL <https://molaison.github.io/MantaID/>

Imports

ggplot2,data.table,magrittr,stringr,tibble,tidyr,tidyselect,ggcorrplot,reshape2,scutr,paradox,RColorBrewer,purrr,dplyr

Suggests mlr3hyperband,mlr3learners,ranger,rpart,xgboost

NeedsCompilation no

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Example	<i>ID example dataset.</i>
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Description

ID example dataset.

Usage

Example

Format

A tibble with 5000 rows and 2 variables.

ID A identifier character.

class The database the ID belongs to.

mi	<i>A wrapper function that executes MantaID workflow.</i>
----	---

Description

A wrapper function that executes MantaID workflow.

Usage

```
mi(
  cores = NULL,
  levels = c("*", 0:9, letters, LETTERS, "_", ".", "-", " ", "/", "\\ ", ":"),
  ratio = 0.3,
  para_blc = FALSE,
  model_path = NULL,
  batch_size = 128,
  epochs = 64,
  validation_split = 0.3,
  graph_path = NULL
)
```

Arguments

cores	The number of cores used when balancing data.
levels	The vector that includes all the single characters occurred in IDs.
ratio	The ratio of the test set.
para_blc	A logical value whether using parallel computing when balancing data.
model_path	The path to save models.
batch_size	The batch size of deep learning model fitting.
epochs	The epochs of deep learning model fitting.
validation_split	The validation ratio of deep learning model fitting.
graph_path	The path to save graphs.

Value

The list of models and graphs.

mi_balance_data	<i>Data balance. Most classes adopt random undersampling, while a few classes adopt smote method to oversample to obtain relatively balanced data.</i>
-----------------	--

Description

Data balance. Most classes adopt random undersampling, while a few classes adopt smote method to oversample to obtain relatively balanced data.

Usage

```
mi_balance_data(data, ratio = 0.3, parallel = FALSE)
```

Arguments

data	A data frame. Except for class column, all are numeric types.
ratio	Numeric between 0 and 1. The percent of the test set split from data.
parallel	Logical.

Value

A list contains a train set and a test set.

mi_clean_data	<i>Reshape data and delete meaningless rows.</i>
---------------	--

Description

Reshape data and delete meaningless rows.

Usage

```
mi_clean_data(data, cols = everything(), placeholder = c("-"))
```

Arguments

data	A dataframe or tibble or data.table or matrix. Names of the column will be regard as the class of ID included in column.
cols	Character vectors. Columns of data that contain the IDs
placeholder	Character vectors. IDs included in placeholder will be omitted.

Value

A tibble with two columns("ID" and "class")

Examples

```
data <- tibble::tibble(  
  "class1" = c("A", "B", "C", "D"),  
  "class2" = c("E", "F", "G", "H"),  
  "class3" = c("L", "M", "-", "O")  
)  
mi_clean_data(data)
```

mi_data_attributes	<i>ID-related datasets in biomed.</i>
--------------------	---------------------------------------

Description

ID-related datasets in biomed.

Usage

```
mi_data_attributes
```

Format

A dataframe with 65 variables and 3 variables.

name The name of dataset.

description Description of dataset.

page collection of attributes.

mi_data_procID	<i>Processed ID data.</i>
----------------	---------------------------

Description

Processed ID data.

Usage

```
mi_data_procID
```

Format

A tibble dataframe with 5000 rows and 21 variables.

pos1 to pos20 Splited ID.

class The databases that ID belongs to.

mi_data_rawID	<i>ID dataset for testing.</i>
---------------	--------------------------------

Description

ID dataset for testing.

Usage

```
mi_data_rawID
```

Format

A tibble with 5000 rows and 2 variables.

ID A identifier character.

class The database the ID belongs to.

mi_filter_feat	<i>Performing feature selection in a automatic way based on correlation and feature importance.</i>
----------------	---

Description

Performing feature selection in a automatic way based on correlation and feature importance.

Usage

```
mi_filter_feat(data, cor_thresh = 0.7, imp_thresh = 0.99, union = FALSE)
```

Arguments

data	The data frame returned by <code>mi_to_numer()</code> .
cor_thresh	The threshold set for Pearson correlation. If correlation value is over this threshold, the two features will be viewed as redundant and one of them will be removed.
imp_thresh	The threshold set for feature importance. The last several features with the lowest importance will be removed if remained importance lower than <code>imp_thresh</code> .
union	The method for combining the decisions of correlation method and importance method. If TRUE, any of the features calculated by the two methods will be returned. Otherwise, only features in the results of both methods will be returned.

Value

The names of the features that should be removed.

mi_get_confusion	<i>Compute the confusion matrix for the predicted result.</i>
------------------	---

Description

Compute the confusion matrix for the predicted result.

Usage

```
mi_get_confusion(result_list, ifnet = FALSE)
```

Arguments

result_list	A list returned from model training functions.
ifnet	Logical. Whether the data is obtained by a deep learning model.

Value

A confusionMatrix object.

mi_get_ID	<i>Get ID data from the Biomart database using attributes.</i>
-----------	--

Description

Get ID data from the Biomart database using attributes.

Usage

```
mi_get_ID(  
  attributes,  
  biomart = "genes",  
  dataset = "hsapiens_gene_ensembl",  
  mirror = "asia"  
)
```

Arguments

attributes	A dataframe. The information we want to retrieve. Use mi_get_ID_attr to have a try.
biomart	BioMart database name you want to connect to. Use biomaRt::listEnsembl to retrieve the possible database names.
dataset	Datasets of the selected BioMart database.
mirror	Specify an Ensembl mirror to connect to.

Value

A tibble dataframe.

mi_get_ID_attr	<i>Get ID attributes from the Biomart database.</i>
----------------	---

Description

Get ID attributes from the Biomart database.

Usage

```
mi_get_ID_attr(  
  biomart = "genes",  
  dataset = "hsapiens_gene_ensembl",  
  mirror = "asia"  
)
```

Arguments

biomart	BioMart database name you want to connect to. Use <code>biomaRt::listEnsembl</code> to retrieve the possible database names.
dataset	Datasets of the selected BioMart database.
mirror	Specify an Ensembl mirror to connect to.

Value

A dataframe.

mi_get_importance	<i>Plot the bar plot for feature importance.</i>
-------------------	--

Description

Plot the bar plot for feature importance.

Usage

```
mi_get_importance(data)
```

Arguments

data	A table.
------	----------

Value

A bar plot.

mi_get_miss	<i>Observe the distribution of the false response of the test set.</i>
-------------	--

Description

Observe the distribution of the false response of the test set.

Usage

```
mi_get_miss(predict)
```

Arguments

predict	An R6 class PredictionClassif.
---------	--------------------------------

Value

A tibble data frame that records the number of wrong predictions for each category ID

mi_get_padlen	<i>Get max length of ID data.</i>
---------------	-----------------------------------

Description

Get max length of ID data.

Usage

```
mi_get_padlen(data)
```

Arguments

data	A dataframe.
------	--------------

Value

An int object.

Examples

```
data(mi_data_rawID)
mi_get_padlen(mi_data_rawID)
```

mi_plot_cor	<i>Plot correlation heatmap.</i>
-------------	----------------------------------

Description

Plot correlation heatmap.

Usage

```
mi_plot_cor(data, cls = "class")
```

Arguments

- data Data frame including IDs' position features.
- cls The name of the class column.

Value

A heatmap.

Examples

```
data(mi_data_procID)
data_num <- mi_to_numer(mi_data_procID)
mi_plot_cor(data_num)
```

mi_plot_heatmap	<i>Plot heatmap for result confusion matrix.</i>
-----------------	--

Description

Plot heatmap for result confusion matrix.

Usage

```
mi_plot_heatmap(table, name = NULL, filepath = NULL)
```

Arguments

- table A table.
- name Model names.
- filepath File path the plot to save. Default NULL.

Value

A ggplot object.

mi_predict_new	<i>Predict new data with a trained learner.</i>
----------------	---

Description

Predict new data with a trained learner.

Usage

```
mi_predict_new(data, result, ifnet = F)
```

Arguments

data	A dataframe.
result	The result object from a previous training.
ifnet	A boolean indicating if a neural network is used for prediction.

Value

A data frame that contains features and 'predict' class.

mi_run_bmr	<i>Compare classification models with small samples.</i>
------------	--

Description

Compare classification models with small samples.

Usage

```
mi_run_bmr(data, row_num = 1000, resamplings = rsmps("cv", folds = 10))
```

Arguments

data	A tibble. All are numeric except the first column is a factor.
row_num	The number of samples used.
resamplings	R6/Resampling. Resampling method.

Value

A list of R6 class of benchmark results and scores of test set. examples `data(mi_data_procID)`
`mi_run_bmr(mi_data_procID)`

mi_split_col	<i>Cut the string of ID column character by character and divide it into multiple columns.</i>
--------------	--

Description

Cut the string of ID column character by character and divide it into multiple columns.

Usage

```
mi_split_col(data, cores = NULL, pad_len = 10)
```

Arguments

data	Dataframe(tibble) to be split.
cores	Int.The num of cores to allocate for computing.
pad_len	The length of longest id, i.e. the maxlength.

Value

A tibble with pad_len+1 column.

mi_split_str	<i>Split the string into individual characters and complete the character vector to the maximum length.</i>
--------------	---

Description

Split the string into individual characters and complete the character vector to the maximum length.

Usage

```
mi_split_str(str, pad_len)
```

Arguments

str	The string to be splited.
pad_len	The length of longest ID, i.e. the maxlength.

Value

Splited character vector.

Examples

```
string_test <- "Good Job"
length <- 15
mi_split_str(string_test, length)
```

mi_to_numer	<i>Convert data to numeric, and for the ID column convert with fixed levels.</i>
-------------	--

Description

Convert data to numeric, and for the ID column convert with fixed levels.

Usage

```
mi_to_numer(
  data,
  levels = c("?", 0:9, letters, LETTERS, "_", ".", "-", " ", "/", "\\ ", ":")
)
```

Arguments

data	A tibble with n position column(pos1,pos2,...) and class column.
levels	Characters accommodated in IDs.

Value

A numeric data frame with numerical or factor type columns.

Examples

```
data(mi_data_procID)
mi_to_numer(mi_data_procID)
```

mi_train_BP	<i>Train a three layers neural network model.</i>
-------------	---

Description

Train a three layers neural network model.

Usage

```
mi_train_BP(
  train,
  test,
  cls = "class",
  path2save = NULL,
  batch_size = 128,
  epochs = 64,
  validation_split = 0.3,
  verbose = 0
)
```

Arguments

train	A dataframe with the class column as label.
test	A dataframe with the class column as label.
cls	A character. The name of the label column.
path2save	The folder path to store the model and train history.
batch_size	Integer or NULL. The number of samples per gradient update.
epochs	The number of epochs to train the model.
validation_split	Float between 0 and 1. Fraction of the training data to be used as validation data.
verbose	The verbosity mode.

Value

A list object containing the prediction confusion matrix, the model object, and the mapping of predicted numbers to classes.

mi_train_rg	<i>Random Forest Model Training.</i>
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Description

Random Forest Model Training.

Usage

```
mi_train_rg(train, test, measure = msr("classif.acc"), instance = NULL)
```

Arguments

train	A dataframe.
test	A dataframe.
measure	Model evaluation method.
instance	A tuner.

Value

A list of learner for predicting and predicted result of test set.

mi_train_rp	<i>Classification tree model training.</i>
-------------	--

Description

Classification tree model training.

Usage

```
mi_train_rp(train, test, measure = msr("classif.acc"), instance = NULL)
```

Arguments

train	A dataframe.
test	A dataframe.
measure	Model evaluation method. Use <code>mlr_measures</code> and <code>msr()</code> to view and choose metrics.
instance	A tuner.

Value

A list of learner for predicting and predicted result of test set.

mi_train_xgb	<i>Xgboost model training</i>
--------------	-------------------------------

Description

Xgboost model training

Usage

```
mi_train_xgb(train, test, measure = msr("classif.acc"), instance = NULL)
```

Arguments

train	A dataframe.
test	A dataframe.
measure	Model evaluation method.
instance	A tuner.

Value

A list of learner for predicting and predicted result of test set.

mi_tune_rg

Tune the Random Forest model by hyperband.

Description

Tune the Random Forest model by hyperband.

Usage

```
mi_tune_rg(
  data,
  resampling = rsmp("cv", folds = 5),
  measure = msr("classif.acc"),
  eta = 3
)
```

Arguments

data	A tibble. All are numeric except the first column is a factor.
resampling	R6/Resampling.
measure	Model evaluation method. Use <code>mlr_measures</code> and <code>msr()</code> to view and choose metrics.
eta	The percent parameter configurations discarded.

Value

A list of tuning instance and stage plot.

mi_tune_rp

Tune the Decision Tree model by hyperband.

Description

Tune the Decision Tree model by hyperband.

Usage

```
mi_tune_rp(
  data,
  resampling = rsmp("bootstrap", ratio = 0.8, repeats = 5),
  measure = msr("classif.acc"),
  eta = 3
)
```


Arguments

data	A tibble. All are numeric except the first column is a factor.
resampling	R6/Resampling.
measure	Model evaluation method. Use <code>mlr_measures</code> and <code>msr()</code> to view and choose metrics.
eta	The percent parameter configurations discarded.

Value

A list of tuning instance and stage plot.

mi_tune_xgb	<i>Tune the Xgboost model by hyperband.</i>
-------------	---

Description

Tune the Xgboost model by hyperband.

Usage

```
mi_tune_xgb(  
  data,  
  resampling = rsmp("cv", folds = 5),  
  measure = msr("classif.acc"),  
  eta = 3  
)
```

Arguments

data	A tibble. All are numeric except the first column is a factor.
resampling	R6/Resampling.
measure	Model evaluation method. Use <code>mlr_measures</code> and <code>msr()</code> to view and choose metrics.
eta	The percent parameter configurations discarded.

Value

A list of tuning instance and stage plot.

mi_unify_mod	<i>Predict with four models and unify results by the sub-model's specificity score to the four possible classes.</i>
--------------	--

Description

Predict with four models and unify results by the sub-model's specificity score to the four possible classes.

Usage

```
mi_unify_mod(  
  data,  
  col_id,  
  result_rg,  
  result_rp,  
  result_xgb,  
  result_BP,  
  c_value = 0.75,  
  pad_len = 30  
)
```

Arguments

data	A dataframe contains the ID column.
col_id	The name of ID column.
result_rg	The result from the Random Forest model.
result_rp	The result from the Decision Tree model.
result_xgb	The result from the XGBoost model.
result_BP	The result from the Backpropagation Neural Network model.
c_value	A numeric value used in the final prediction calculation.
pad_len	The length to pad the ID characters to.

Value

A dataframe.

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