## Package 'TidyML'

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```
Title Machine Learning Modelling For Everyone
Version 0.0.0.9000
Description
      TidyML is a minimal library focused on providing all the essential tools for the workflow of a
      machine learning modelling process. The whole process is divided into 5 steps:
      preprocessing() -> build_model() -> fine_tuning() -> show_results() -> sensitivity_analysis()
License `use_mit_license()`, `use_gpl3_license()` or friends to pick a
      license
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```

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```
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URL https://github.com/JMartinezGarcia/TidyML

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build\_model

Create ML Model

#### **Description**

Create ML Model

## Usage

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```
build_model(analysis_object, model_name, hyperparameters = NULL)
```

## Arguments

analysis\_object

analysis\_object created from preprocessing function.

model\_name

Name of the ML Model. A string of the model name: "Neural Network", "Random Forest", "SVM" or "XGBOOST".

hyperparameters

Hyperparameters of the ML model. List containing the name of the hyperparameter and its value or range of values.

## Value

Updated analysis\_object

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#### Hyperparameters

#### **Neural Network:**

Parsnip model using **brulee** engine. Hyperparameters:

• hidden\_units: Number of Hidden Neurons. A single value, a vector with range values c(min\_val, max\_val) or NULL for default range c(5, 20).

- activation: Activation Function. A vector with any of ("relu", "sigmoid", "tanh") or NULL for default values c("relu", "sigmoid", "tanh").
- learn\_rate: Learning Rate. A single value, a vector with range values c(min\_val, max\_val) or NULL for default range c(-3, -1) in log10 scale.

#### **Random Forest:**

Parsnip model using **ranger** engine. Hyperparameters:

- **trees**: Number of Trees. A single value, a vector with range values c(min\_val, max\_val). Default range c(100, 300).
- mtry: Number of variables randomly selected as candidates at each split. A single value, a vector with range values c(min\_val, max\_val) or NULL for default range c(3, 8).
- min\_n: Minimum Number of samples to split at each node. A single value, a vector with range values c(min\_val, max\_val) or NULL for default range c(2, 25).

#### **XGBOOST:**

Parsnip model using **xgboost** engine. Hyperparameters:

- **trees**: Number of Trees. A single value, a vector with range values c(min\_val, max\_val) or NULL for default range c(100, 300).
- mtry: Number of variables randomly selected as candidates at each split. A single value, a vector with range values c(min\_val, max\_val) or NULL for default range c(3, 8).
- min\_n: Minimum Number of samples to split at each node. A single value, a vector with range values c(min\_val, max\_val) or NULL for default range c(5, 25).
- **tree\_depth**: Maximum tree depth. A single value, a vector with range values c(min\_val, max\_val) or NULL for default range c(3, 10).
- learn\_rate: Learning Rate. A single value, a vector with range values c(min\_val, max\_val) or NULL for default range c(-4, -1) in log10 scale.
- loss\_reduction: Minimum loss reduction required to make a further partition on a leaf node. A single value, a vector with range values c(min\_val, max\_val) or NULL for default range c(-5, 1.5) in log10 scale.

#### SVM:

Parsnip model using kernlab engine. Hyperparameters:

- **cost**: Penalty parameter that regulates model complexity and misclassification tolerance. A single value, a vector with range values c(min\_val, max\_val) or NULL for default range c(-3, 3) in log10 scale.
- margin: Distance between the separating hyperplane and the nearest data points. A single value, a vector with range values c(min\_val, max\_val) or NULL for default range c(0, 0.2).
- type: Kernel to be used. A single value from ("linear", "rbf", "polynomial")
- **rbf\_sigma**: A single value, a vector with range values c(min\_val, max\_val) or NULL for default range c(-5, 0) in log10 scale.
- **degree**: Polynomial Degree (polynomial kernel only). A single value, a vector with range values c(min\_val, max\_val) or NULL for default range c(1, 3).
- scale\_factor: Scaling coefficient applied to inputs. (polynomial kernel only) A single value, a vector with range values c(min\_val, max\_val) or NULL for default range c(-5, -1) in log10 scale.

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fine\_tuning

Fine Tune ML Model

#### **Description**

Fine Tune ML Model

#### Usage

fine\_tuning(analysis\_object, tuner, metrics, plot\_results = F, verbose = FALSE)

#### **Arguments**

analysis\_object

analysis\_object created from build\_model function.

tuner Name of the Hyperparameter Tuner. A string of the tuner name: "Bayesian

Optimization" or "Grid Search CV".

metrics Metric used for Model Selection. A string of the name of metric (see Metrics).

plot\_results Whether to plot the tuning results. Boolean TRUE or FALSE (default). verbose Whether to show tuning process. Boolean TRUE or FALSE (default).

#### Value

Updated analysis\_object

#### **Tuners**

## **Bayesian Optimization:**

• Initial data points: 20

• Maximum number of iterations: 25

• Convergence after 5 iterations without improvement

• Train / Validation / Test: 0.6 / 0.2 / 0.2

#### **Grid Search CV:**

• Number of Folds: 5

• Maximum levels per hyperparameter: 10

• Train / Test: 0.75 / 0.25

## Metrics

## **Regression Metrics:**

- rmse
- mae
- mpe
- mape
- ccc
- smape
- rpiq

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• rsq

#### **Classification Metrics:**

- accuracy
- bal\_accuracy
- recall
- sensitivity
- specificity
- kap
- f\_meas
- mcc
- j\_index
- detection\_prevelance
- roc\_auc
- pr\_auc
- gain\_capture
- brier\_class
- roc\_aunp

preprocessing

Preprocessing Data Matrix

#### **Description**

Preprocessing Data Matrix

## Usage

```
preprocessing(
   df,
   formula,
   task = "regression",
   num_vars = NULL,
   cat_vars = NULL,
   norm_num_vars = "all",
   encode_cat_vars = "all",
   y_levels = NULL
)
```

## **Arguments**

df Input DataFrame. Either a data.frame or tibble.

formula Modelling Formula. A string of characters or formula.

task Modelling Task. Either "regression" or "classification".

num\_vars Optional vector of names of the numerical features.

cat\_vars Optional vector of names of the categorical features.

norm\_num\_vars Normalize numeric features as z-scores. Either vector of names of numerical

features to be normalized or "all" (default).

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encode\_cat\_vars

One Hot Encode Categorical Features. Either vector of names of categorical

features to be encoded or "all" (default).

y\_levels Optional ordered vector with names of the target variable levels (Classification

task only).

#### Value

An analysis\_object

sensitivity\_analysis Perform Sensitivity Analysis and Interpretable ML methods

#### **Description**

Perform Sensitivity Analysis and Interpretable ML methods

#### Usage

```
sensitivity_analysis(analysis_object, methods = c("PFI"), metric = NULL)
```

## **Arguments**

analysis\_object

analysis\_object created from fine\_tuning function.

methods Method to be used. A string of the method name: "PFI" (Permutation Feature

Importance), "SHAP" (SHapley Additive exPlanations), "Integrated Gradients"

(Neural Network only) or "Olden" (Neural Network only).

metric Metric used for "PFI" method (Permutation Feature Importance). A string of the

name of metric (see Metrics).

## Value

Updated analysis\_object

show\_results

Showcase Summary Results and Plots

#### Description

Showcase Summary Results and Plots

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#### Usage

```
show_results(
    analysis_object,
    summary = FALSE,
    roc_curve = FALSE,
    pr_curve = FALSE,
    gain_curve = FALSE,
    lift_curve = FALSE,
    dist_by_class = FALSE,
    reliability_plot = FALSE,
    confusion_matrix = FALSE,
    scatter_residuals = FALSE,
    scatter_predictions = FALSE,
    residuals_dist = FALSE,
    new_data = "test"
)
```

#### **Arguments**

analysis\_object

analysis\_object created from fine\_tuning function.

summary Whether to plot summary results table. Boolean (FALSE by default).

roc\_curve Whether to plot ROC Curve (Classification task only). Boolean (FALSE by

default).

pr\_curve Whether to plot ROC Curve (Classification task only). Boolean (FALSE by

default).

gain\_curve Whether to plot ROC Curve (Classification task only). Boolean (FALSE by

default).

lift\_curve Whether to plot ROC Curve (Classification task only). Boolean (FALSE by

default).

dist\_by\_class Whether to plot distribution of output probability by class (Classification task

only). Boolean (FALSE by default).

reliability\_plot

Whether to plot Reliability Plot (Binary Classification task only). Boolean (FALSE by default).

confusion\_matrix

Whether to Confusion Matrix (Classification task only). Boolean (FALSE by default)

scatter\_residuals

Whether to plot Residuals vs Predictions (Regression task only). Boolean (FALSE by default).

scatter\_predictions

Whether to plot Predictions vs Observed (Regression task only). Boolean (FALSE by default).

residuals\_dist Whether to plot Residuals Distribution (Regression task only). Boolean (FALSE by default).

new\_data Data to be used for Confusion Matrix, Reliability Plot, Distribution by Class Plot, Residuals vs Predictions Plot, Predictions vs Observed Plot and Residuals

Distribution Plot. A string with the name of the data\_set: "train", "validation",

"test" (default) or "all".

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#### Value

Updated analysis\_object

sim\_data

Example Data Set

#### **Description**

This dataset contains simulated data of a psychometric trial.

## Usage

sim\_data

#### **Format**

A data frame with 1000 rows and 10 columns:

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