goophi - classification

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1 Introduction

1) 본 문서는 goophi 패키지를 Shiny app에서 사용하는 것을 상정해 작성했습니다.

2) 본 문서의 케이스 스타일은 Camel case와 Snake case가 혼용되어 있습니다.

- Camel case : goophi의 함수명 및 파라미터명
- Snake case: 유저로부터 받는 입력, shiny app의 server에서 사용(될 것이라고 예상)하는 object명, snake case로 작성된 dependencies의 함수명 등

2 Import sample data

1) 전처리가 완료된 샘플데이터를 불러옵니다.

- NA가 없어야 함
- string value가 있는 열은 factor로 변환
- 한 열이 모두 같은 값으로 채워져 있을 경우 제외해야 함
- Date type column이 없어야 함
- Outcome 변수는 classification의 경우 factor, regression의 경우 numeric이어야 함 (clustering은 outcome변수를 사용하지 않음)

```
library(goophi)

cleaned_data <- read.csv(file = "~/git/goophi/data/boston_c.csv",
                         stringsAsFactors = TRUE
                         )
cleaned_data$Pcrime <- as.factor(cleaned_data$Pcrime)
str(cleaned_data)
```

```
'data.frame':   506 obs. of  14 variables:
 $ zn     : num  18 0 0 0 0 0 12.5 12.5 12.5 12.5 ...
 $ indus  : num  2.31 7.07 7.07 2.18 2.18 2.18 7.87 7.87 7.87 7.87 ...
 $ chas   : Factor w/ 2 levels "otherwise","Tract bounds river": 1 1 1 1 1 1 1 1 1 1 ...
 $ nox    : num  0.538 0.469 0.469 0.458 0.458 0.458 0.524 0.524 0.524 0.524 ...
 $ rm     : num  6.58 6.42 7.18 7 7.15 ...
 $ age    : num  65.2 78.9 61.1 45.8 54.2 58.7 66.6 96.1 100 85.9 ...
 $ dis    : num  4.09 4.97 4.97 6.06 6.06 ...
 $ rad    : int  1 2 2 3 3 3 5 5 5 5 ...
 $ tax    : int  296 242 242 222 222 222 311 311 311 311 ...
 $ ptratio: num  15.3 17.8 17.8 18.7 18.7 18.7 15.2 15.2 15.2 15.2 ...
 $ black  : num  397 397 393 395 397 ...
 $ lstat  : num  4.98 9.14 4.03 2.94 5.33 ...
 $ medv   : num  24 21.6 34.7 33.4 36.2 28.7 22.9 27.1 16.5 18.9 ...
 $ Pcrime : Factor w/ 2 levels "0","1": 1 1 1 1 1 1 1 1 1 1 ...
```

3 Data Setup Tab

User Input	description
target_var	목적 변수
train_set_ratio	전체 데이터 중 train set의 비율 (range: 0.0 – 1.0)

1) User input을 다음과 같이 받습니다.

- formula는 user가 target_var를 입력할 때 함께 생성되도록 함

```
target_var <- "Pcrime"
train_set_ratio <- "0.7"
seed <- "1234"
formula <- paste0(target_var, " ~ .")
```

2) Train-test split 작업이 완료된 Object를 저장하고, Train set을 보여줍니다.

```
split_tmp <- goophi::trainTestSplit(data = cleaned_data,
                                    target = target_var,
                                    prop = train_set_ratio,
                                    seed = seed
                                    )

data_train <- split_tmp[[1]] # train data
data_test <- split_tmp[[2]] # test data
data_split <- split_tmp[[3]] # whole data with split information
```

3) train set에 적용할 전처리 정보를 담은 recipe를 생성합니다

```
rec <- goophi::prepForCV(data = data_train,
                         formula = formula,
                         seed = seed
                         )
```

4 Modeling Tab

User Input	description
algo	ML 알고리즘 선택
engine	engine 선택
mode	mode 선택
metric	Best performance에 대한 평가지표 선택
v	Cross validation시 train set을 몇 번 분할할 것인지 입력
...	각 모델의 hyperparameter의 최소/최대값(Min, Max), 몇 단계로 나눌지(Levels)

모델 object를 저장할 빈 리스트를 생성합니다.

```
models_list <- list()
```

4.1 Logistic Regression

```
# User input

mode <- "classification"
algo <- "logisticRegression"
engine <- "glmnet" # glmnet (default), glm, stan

penalty_range_min <- "0.001"
penalty_range_max <- "1.0"
penalty_range_levels <- "5"
mixture_range_min <- "0.0"
mixture_range_max <- "1.0"
mixture_range_levels <- "5"

v <- "2"

metric <- "roc_auc" # roc_auc (default), accuracy

# Modeling

finalized <- goophi::logisticRegression(
  algo = algo,
  engine = engine,
  mode = mode,
  trainingData = data_train,
```

```
  splitedData = data_split,
  formula = formula,
  rec = rec,
  v = v,
  penaltyRangeMin = penalty_range_min,
  penaltyRangeMax = penalty_range_max,
  penaltyRangeLevels = penalty_range_levels,
  mixtureRangeMin = mixture_range_min,
  mixtureRangeMax = mixture_range_max,
  mixtureRangeLevels = mixture_range_levels,
  metric = metric
)

# Add the model to models_list
models_list[[paste0(algo, "_", engine)]] <- finalized$finalFittedModel
```

4.2 K Nearest Neighbor

```
# User input

mode <- "classification"
algo <- "KNN"
engine <- "kknn" # kknn (defualt)

neighbors_range_min <- "1"
neighbors_range_max <- "10"
neighbors_range_levels <- "10"

v <- "2"

metric <- "roc_auc" # roc_auc (default), accuracy

# Modeling

finalized <- goophi::KNN(
  algo = algo,
  engine = engine,
  mode = mode,
  trainingData = data_train,
  splitedData = data_split,
```

```
  formula = formula,
  rec = rec,
  v = v,
  neighborsRangeMin = neighbors_range_min,
  neighborsRangeMax = neighbors_range_max,
  neighborsRangeLevels = neighbors_range_levels,
  metric = metric
)

# Add the model to models_list
models_list[[paste0(algo, "_", engine)]] <- finalized$finalFittedModel
```

4.3 Naive Bayes

```
# User input

mode <- "classification"
algo <- "naiveBayes"
engine <- "klaR" # klaR (default), naivebayes

smoothness_range_min <- "0.5"
smoothness_range_max <- "1.5"
smoothness_range_levels <- "3"
laplace_range_min <- "0.0"
laplace_range_max <- "3.0"
laplace_range_levels <- "4"

v <- "2"

metric <- "roc_auc" # roc_auc (default), accuracy

# Modeling

finalized <- goophi::naiveBayes(
  algo = algo,
  engine = engine,
  mode = mode,
  trainingData = data_train,
  splitedData = data_split,
  formula = formula,
```

```
  rec = rec,
  v = v,
  smoothnessRangeMin = smoothness_range_min,
  smoothnessRangeMax = smoothness_range_max,
  smoothnessRangeLevels = smoothness_range_levels,
  LaplaceRangeMin = laplace_range_min,
  LaplaceRangeMax = laplace_range_max,
  LaplaceRangeLevels = laplace_range_levels,
  metric = metric
)

# Add the model to models_list
models_list[[paste0(algo, "_", engine)]] <- finalized$finalFittedModel
```

4.4 Decision Tree

```
# User input

mode <- "classification"
algo <- "decisionTree"
engine <- "rpart" # rpart (default), C5.0, partykit

tree_depth_range_min <- "1"
tree_depth_range_max <- "15"
tree_depth_range_levels <- "3"
min_n_range_min <- "2"
min_n_range_max <- "40"
min_n_range_levels <- "3"
cost_complexity_range_min <- "-2.0"
cost_complexity_range_max <- "-1.0"
cost_complexity_range_levels <- "2"

v <- "2"

metric <- "roc_auc" # roc_auc (default), accuracy

# Modeling

finalized <- goophi::decisionTree(
  algo = algo,
```

```
  engine = engine,
  mode = mode,
  trainingData = data_train,
  splitedData = data_split,
  formula = formula,
  rec = rec,
  v = v,
  treeDepthRangeMin = tree_depth_range_min,
  treeDepthRangeMax = tree_depth_range_max,
  treeDepthRangeLevels = tree_depth_range_levels,
  minNRangeMin = min_n_range_min,
  minNRangeMax = min_n_range_max,
  minNRangeLevels = min_n_range_levels,
  costComplexityRangeMin = cost_complexity_range_min,
  costComplexityRangeMax = cost_complexity_range_max,
  costComplexityRangeLevels = cost_complexity_range_levels,
  metric = metric
)

# Add the model to models_list
models_list[[paste0(algo, "_", engine)]] <- finalized$finalFittedModel
```

4.5 Random Forest

```
# User input

mode <- "classification"
algo <- "randomForest"
engine <- "ranger" # ranger (default), randomForest, partykit

mtry_range_min <- "1"
mtry_range_max <- "20"
mtry_range_levels <- "3"
trees_range_min <- "100"
trees_range_max <- "1000"
trees_range_levels <- "3"
min_n_range_min <- "2"
min_n_range_max <- "40"
min_n_range_levels <- "3"
```

```r
v <- "2"

metric <- "roc_auc" # roc_auc (default), accuracy

# Modeling

finalized <- goophi::randomForest(
  algo = algo,
  engine = engine,
  mode = mode,
  trainingData = data_train,
  splitedData = data_split,
  formula = formula,
  rec = rec,
  v = v,
  mtryRangeMin = mtry_range_min,
  mtryRangeMax = mtry_range_max,
  mtryRangeLevels = mtry_range_levels,
  treesRangeMin = trees_range_min,
  treesRangeMax = trees_range_max,
  treesRangeLevels = trees_range_levels,
  minNRangeMin = min_n_range_min,
  minNRangeMax = min_n_range_max,
  minNRangeLevels = min_n_range_levels,
  metric = metric
)

# Add the model to models_list
models_list[[paste0(algo, "_", engine)]] <- finalized$finalFittedModel
```

4.6 XGBoost

```r
# User input

mode <- "classification"
algo <- "XGBoost"
engine <- "xgboost" # xgboost

tree_depth_range_min <- "5"
tree_depth_range_max <- "15"
```

```
tree_depth_range_levels <- "3"
trees_range_min <- "8"
trees_range_max <- "32"
trees_range_levels <- "3"
learn_rate_range_min <- "-2.0"
learn_rate_range_max <- "-1.0"
learn_rate_range_levels <- "2"
mtry_range_min <- "0.0"
mtry_range_max <- "1.0"
mtry_range_levels <- "3"
min_n_range_min <- "2"
min_n_range_max <- "40"
min_n_range_levels <- "3"
loss_reduction_range_min <- "-1.0"
loss_reduction_range_max <- "1.0"
loss_reduction_range_levels <- "3"
sample_size_range_min <- "0.0"
sample_size_range_max <- "1.0"
sample_size_range_levels <- "3"
stop_iter <- "30"

v <- "2"

metric <- "roc_auc" # roc_auc (default), accuracy

# Modeling

finalized <- goophi::xgBoost(
  algo = algo,
  engine = engine,
  mode = mode,
  trainingData = data_train,
  splitedData = data_split,
  formula = formula,
  rec = rec,
  v = v,
  treeDepthRangeMin = tree_depth_range_min,
  treeDepthRangeMax = tree_depth_range_max,
  treeDepthRangeLevels = tree_depth_range_levels,
  treesRangeMin = trees_range_min,
  treesRangeMax = trees_range_max,
  treesRangeLevels = trees_range_levels,
```

```
  learnRateRangeMin = learn_rate_range_min,
  learnRateRangeMax = learn_rate_range_max,
  learnRateRangeLevels = learn_rate_range_levels,
  mtryRangeMin = mtry_range_min,
  mtryRangeMax = mtry_range_max,
  mtryRangeLevels = mtry_range_levels,
  minNRangeMin = min_n_range_min,
  minNRangeMax = min_n_range_max,
  minNRangeLevels = min_n_range_levels,
  lossReductionRangeMin = loss_reduction_range_min,
  lossReductionRangeMax = loss_reduction_range_max,
  lossReductionRangeLevels = loss_reduction_range_levels,
  sampleSizeRangeMin = sample_size_range_min,
  sampleSizeRangeMax = sample_size_range_max,
  sampleSizeRangeLevels = sample_size_range_levels,
  stopIter = stop_iter,
  metric = metric
)

# Add the model to models_list
models_list[[paste0(algo, "_", engine)]] <- finalized$finalFittedModel
```

4.7 lightGBM

4.8 MLP

```
# User input

mode <- "classification"
algo <- "MLP"
engine <- "nnet" # nnet

hidden_units_range_min <- "1"
hidden_units_range_max <- "10"
hidden_units_range_levels <- "3"
penalty_range_min <- "0.001"
penalty_range_max <- "1.0"
penalty_range_levels <- "3"
epochs_range_min <- "10"
epochs_range_max <- "100"
```

```
epochs_range_levels <- "2"

v <- "2"

metric <- "roc_auc" # roc_auc (default), accuracy

# Modeling

finalized <- goophi::MLP(
  algo = algo,
  engine = engine,
  mode = mode,
  trainingData = data_train,
  splitedData = data_split,
  formula = formula,
  rec = rec,
  v = v,
  hiddenUnitsRangeMin = hidden_units_range_min,
  hiddenUnitsRangeMax = hidden_units_range_max,
  hiddenUnitsRangeLevels = hidden_units_range_levels,
  penaltyRangeMin = penalty_range_min,
  penaltyRangeMax = penalty_range_max,
  penaltyRangeLevels = penalty_range_levels,
  epochsRangeMin = epochs_range_min,
  epochsRangeMax = epochs_range_max,
  epochsRangeLevels = epochs_range_levels,
  metric = metric
)

# Add the model to models_list
models_list[[paste0(algo, "_", engine)]] <- finalized$finalFittedModel
```

4.9 Modeling without hyperparameter

함수 내에 기본값을 선언해 뒀기때문에, 유저로부터 입력을 받지 않아도 모델링이 가능합니다. 아래처럼 hyperparameter관련 파라미터, v를 따로 입력받지 않아도 됩니다.

```
# User input

mode <- "classification"
algo <- "LogisticAuto"
```

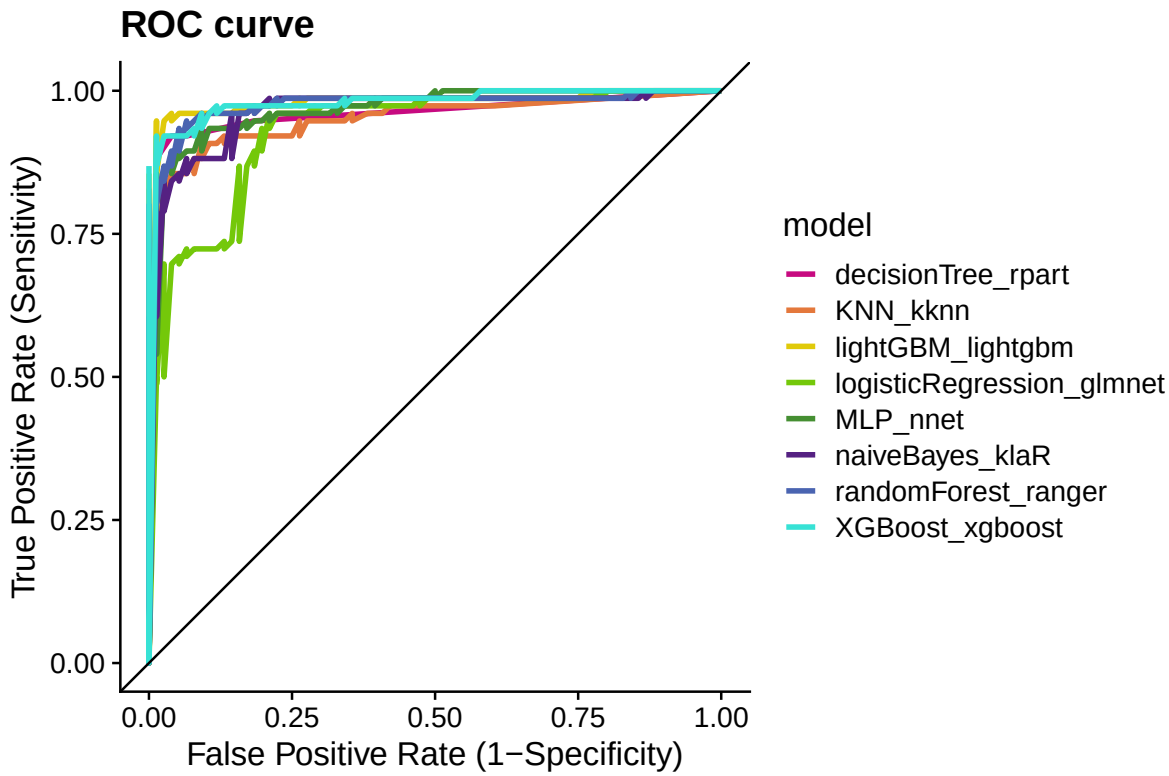
```
engine <- "glmnet" # glmnet (default), glm, stan

metric <- "roc_auc" # roc_auc (default), accuracy

# Modeling

finalized <- goophi::logisticRegression(
  algo = algo,
  engine = engine,
  mode = mode,
  trainingData = data_train,
  splitedData = data_split,
  formula = formula,
  rec = rec,
  # v = v,
  # penaltyRangeMin = penalty_range_min,
  # penaltyRangeMax = penalty_range_max,
  # penaltyRangeLevels = penalty_range_levels,
  # mixtureRangeMin = mixture_range_min,
  # mixtureRangeMax = mixture_range_max,
  # mixtureRangeLevels = mixture_range_levels,
  metric = metric
)
```

5 Sources for report

5.1 ROC Curve

유저가 선택한 모델의 ROC curve 출력

```
roc_curve <- goophi::rocCurve(
  modelsList = models_list,
  targetVar = target_var
)
roc_curve
```



5.2 Confusion Matrix

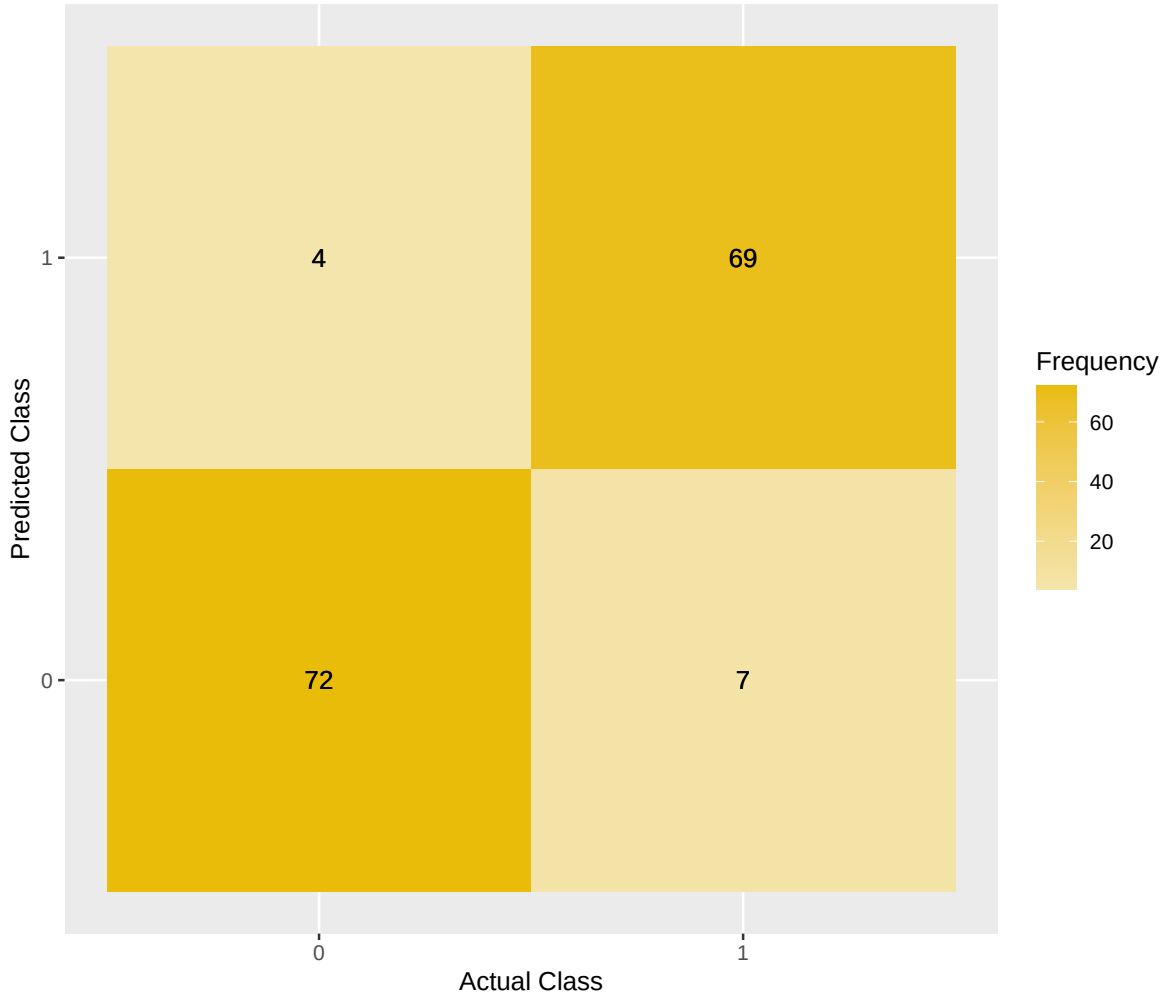
유저가 선택한 모델의 confusion matrix 출력 리스트 내 모델의 이름은 {algo}_{engine}의 형태로 저장되어 있음

```
# User input
names(models_list)
```

```
[1] "logisticRegression_glmnet" "KNN_kknn"
[3] "naiveBayes_klaR"           "decisionTree_rpart"
[5] "randomForest_ranger"       "XGBoost_xgboost"
[7] "lightGBM_lightgbm"         "MLP_nnet"
```

```
model_name <- "randomForest_ranger"
```

```
cm <- goophi::confusionMatrix(
  modelName = model_name,
  modelsList = models_list,
  targetVar = target_var
)
cm
```



5.3 Evaluation metrics

- 모델 성능 비교를 위한 표 출력
- options(yardstick.event_level = “second”)은 오름차순으로 factor의 level 설정하기 위한 옵션

```
options(yardstick.event_level = "second")
evalMet <- goophi::evalMetricsC(models_list, target_var)
knitr::kable(evalMet)
```

	Accuracy	Recall	Specificity	Precision	F1-score	Kappa	MCC
logisticRegression_glmnet	0.816	0.908	0.724	0.767	0.831	0.632	0.643
KNN_kknn	0.895	0.934	0.855	0.866	0.899	0.789	0.792
naiveBayes_klaR	0.901	0.947	0.855	0.867	0.906	0.803	0.806
decisionTree_rpart	0.941	0.961	0.921	0.924	0.942	0.882	0.882
randomForest_ranger	0.928	0.947	0.908	0.911	0.929	0.855	0.856
XGBoost_xgboost	0.954	0.987	0.921	0.926	0.955	0.908	0.910
lightGBM_lightgbm	0.961	0.987	0.934	0.938	0.962	0.921	0.922
MLP_nnet	0.908	0.908	0.908	0.908	0.908	0.816	0.816