The R codes are structured to mirror the experimental setup (see Figure ??). The source codes are divided into the following self-explanatory scripts. These scripts read and train the models on the training sets with various feature selection methods and evaluate their performances on the test sets in an automatical fashion.

R Codes for Regression Tasks

Baseline Learner for Regression

```
# Baseline learners without interactions: regression tasks ----
# Compare baseline learners with other methods
# O. Load packages ----
library(mlr)
library(tidyverse)
# 1. Run baseline learners ----
# Initialise the data frame to store results,
# Prepare data sets and target continuous features
            <- data.frame()
result
data_files <- c('BostonHousing', 'Ailerons', 'Elevators')</pre>
            <- c('medv', 'V41', 'V19')
targets
# Common learner: linear regression
wrapper
            <- makeLearner('regr.lm')
# Loop for each dataset
for(j in 1:length(data_files) ){
  train_data <- read.csv(paste0(data_files[j], '_train.csv'))</pre>
  test_data
              <- read.csv(paste0(data_files[j],'_test.csv'))</pre>
  train_task <- makeRegrTask(data = train_data, target = targets[j])</pre>
  test_task <- makeRegrTask(data = test_data, target = targets[j])</pre>
  baseModel <- train(wrapper, train_task)</pre>
  train pred <- predict(baseModel, train task)</pre>
              <- predict(baseModel, test_task)</pre>
  test_pred
 result[j, 'Data'] <- data_files[j]</pre>
  result[j, 'AIC'] <- AIC(baseModel$learner.model)</pre>
  result[j, 'BIC'] <- BIC(baseModel$learner.model)</pre>
  result[j, 'Train_RMSE'] <- mlr::performance(train_pred, mlr::rmse)</pre>
  result[j, 'Test_RMSE'] <- mlr::performance(test_pred, mlr::rmse)</pre>
}
# Save the result as a csv file
write.csv(result, 'baselearner_regr.csv', row.names = FALSE)
```

Modified Make Regression Task Function

```
#' @description Generating pairwise interaction terms of a data and
# ' pass in to a regression task
#'
```

```
#' Oparam data A data frame containing the features and target variable(s)
#' Oparam target Name of the target variable
#' Oparam order Interaction order. The allowed values are 1, 2, and 3.
                Default is 2L
modifiedMakeRegrTask <- function(data, target, order = 2,</pre>
                                  remove.constant = TRUE,...){
  # Argument check on "order"
  # It is not necessary to check on "data" or "target" as they will
  # be handled by makeClassifTask function
  if( !order %in% c(1, 2, 3) | !inherits(order, 'integer')){
    stop('order must be 1, 2, or 3.')
  # create the classification task
       <- mlr::makeRegrTask(data = data, target = target, ...)</pre>
  if( order %in% c(2, 3)){
    # extract target and descriptive features
    y <- task$env$data[, target]
    if( order == 2){
      fml <- formula(paste0(target, "~.*."))</pre>
    }else{
      fml <- formula(paste0(target, "~.^3"))</pre>
    }
      <- data.frame(model.matrix(fml, task$env$data))</pre>
    # Remove constant terms
    if( remove.constant){
        <- mlr::removeConstantFeatures(X)</pre>
    # bind the data
    newdata <- cbind(X,y)</pre>
    colnames(newdata)[ncol(newdata)] <- target</pre>
    # prompt warning message if p > n
    p \leftarrow ncol(X)
    if( p > nrow(X)){
      warning('More features than number of observations.')
    # reconfigure the task
    task <- mlr::makeRegrTask(data = newdata, target = target, ...)</pre>
  }
```

```
return(task)
}
```

Automatic Feature Selection Script for Regression Tasks

```
# O. Preliminary ----
# Load the relevant packages
library(mlr)
library(spFSR)
library(jsonlite)
library(glinternet)
# Source the modified modified make-regression task with higher orders
source('modifiedMakeRegrTask.R')
# Common learner: linear regression
           <- makeLearner('regr.lm')</pre>
wrapper
# Datasets and number of CV
data_files <- c('BostonHousing', 'Ailerons', 'Elevators')</pre>
          <- c('medv', 'V41', 'V19')
targets
numberCV <-c(4, 10, 10)
# 1. Learning interactions using SFS for linear regresssion task ----
# Define SFS control
SFSctrl <- makeFeatSelControlSequential(method = 'sfs',
                                            alpha = 0.001, beta = -0.0005)
for(j in 1:length(data_files)){
  # Initialise the all_result data.frame to store the result
  m <- 0
  results_summary <- data.frame()</pre>
  data_name <- data_files[j]</pre>
  target <- targets[j]</pre>
  try(
    {
                  <- read.csv(paste0(data_files[j], '_train.csv'))</pre>
      data
      test_data
                 <- read.csv(paste0(data_files[j],'_test.csv'))</pre>
    }
  )
 task <- makeRegrTask(data = data, target = target)</pre>
  # Create a vector of random seeds for reproducibility
  if( data name == 'BostonHousing'){
    seed_vector <- c(1, 1010, 4, 781, 9990, 9999, 81, 46, 67, 2, 3, 1017)
  }else{
    seed_vector <- c(1, 4, 781)
  }
```

```
for(i in 1:length(seed_vector)){
 seed.number <- seed vector[i]</pre>
 set.seed(seed.number)
 m \leftarrow m + 1
  # Resampling
              <- makeResampleDesc(method = 'CV' , iters = numberCV[j])</pre>
 rdesc
  # Extract main effects
 main_sfeats <- selectFeatures(wrapper, task = task, resampling = rdesc,</pre>
                                 control = SFSctrl, show.info = TRUE,
                                 measures = mlr::rmse )
  # Obtain the performance with main effects only
 reduced_main_task <- makeRegrTask(id = 'reduced main',</pre>
                                     data = data[, c(main_sfeats$x , targets[j])],
                                     target = targets[j])
  # Add interactions
  second_task <- modifiedMakeRegrTask(id = 'interaction',</pre>
                                        data = data[, c(main_sfeats$x , target)],
                                        target = target, order = 2L)
  # Specify the maximum number of trials
  success <- FALSE
 tryCatch({
    second_sfeats <- selectFeatures(wrapper, task = second_task,</pre>
                                     resampling = rdesc,
                                     control = SFSctrl, show.info = TRUE,
                                     measures = mlr::rmse)
    success <- TRUE
 },
 error = function(e){conditionMessage(e)}
 results_summary[m, 'dataset']
                                    <- data name
 results_summary[m, 'seed_number'] <- seed.number</pre>
 results_summary[m, 'p_0']
                                      <- length(main_sfeats$x)
  if(exists('second_sfeats')){
                   <- as.character(unique(c(main_sfeats$x , second_sfeats$x)))</pre>
    signif_terms
    results_summary[m, 'p_1'] <- length(signif_terms) - length(main_sfeats$x)
    # Add the omitted main effects
    third_task <- makeRegrTask(id = 'strong hierarchy',
                                data =
                                 second_task$env$data[, c(signif_terms, targets[j])],
```

```
target = targets[j])
                        <- train( wrapper, third_task )
      constrainedMod
      constrainedPred <- predict( constrainedMod, third_task)</pre>
      results_summary[m, 'train_rmse'] <- performance( constrainedPred,</pre>
                                                          measure = mlr::rmse)
      results summary[m, 'train AIC'] <- AIC( constrainedMod$learner.model)
      results_summary[m, 'train_BIC'] <- BIC( constrainedMod$learner.model)</pre>
      sub_test_task <- modifiedMakeRegrTask(data = test_data, target = targets[j],</pre>
                                               order = 2L, remove.constant = FALSE)
      sub_test_task <- makeRegrTask(data =</pre>
                                       sub_test_task$env$data[, c(signif_terms, targets[j])],
                                      target = targets[j], id = 'test_subset')
                                       <- predict(constrainedMod , sub_test_task)</pre>
      sub_pred_test
      results_summary[m, 'test_rmse'] <- performance( sub_pred_test, mlr::rmse)
      output <- list(coeff = constrainedMod$learner.model$coefficients,</pre>
                      result = results_summary[m, ],
                      features = signif_terms)
      write(toJSON(output, auto_unbox = TRUE, pretty = TRUE, factor = 'string'),
            paste0('GA_',data_name,'_',seed.number,'.txt'))
    }else{
      results_summary[m, 'p_1']
      results_summary[m, 'train_rmse'] <- NA</pre>
      results_summary[m, 'train_AIC'] <- NA
      results_summary[m, 'train_BIC'] <- NA</pre>
      results_summary[m, 'test_rmse'] <- NA</pre>
    }
  }
  write.csv(results_summary, paste0('SFS_regr_',data_files[j],'.csv'),
            row.names = FALSE)
}
# 2. Learning interactions via hierarchical group-lasso regularization ----
for(j in 1:length(data_files)){
  # Initialise the all_result data.frame to store the result
  m < -0
  data_name <- data_files[j]</pre>
  all_result <- data.frame()</pre>
```

```
if( data_name == 'BostonHousing'){
  data <- read.csv('BostonHousing_train.csv')</pre>
  data <- removeConstantFeatures(data)</pre>
        <- data$medv
        <- data[, c(1:ncol(data)-1)]
  test_data <- read.csv('BostonHousing_test.csv')</pre>
  test_Y <- test_data$medv</pre>
  test X
          <- test_data[, c(1:ncol(test_data)-1)]</pre>
}else if( data_name == 'Ailerons'){
  data <- read.csv('Ailerons_train.csv')</pre>
  data <- removeConstantFeatures(data)</pre>
        <- data$V41
        <- data[, c(1:ncol(data)-1)]
  test_data <- read.csv('Ailerons_test.csv')</pre>
  test_Y <- test_data$V41</pre>
  \mathsf{test}_{\mathsf{X}}
            <- test_data[, c(1:ncol(test_data)-1)]</pre>
}else if( data_name == 'Elevators'){
  data <- read.csv('Elevators_train.csv')</pre>
  data <- removeConstantFeatures(data)</pre>
         <- data$V19
        <- data[, c(1:ncol(data)-1)]
  test_data <- read.csv('Elevators_test.csv')</pre>
  test_Y <- test_data$V19</pre>
  test_X <- test_data[, c(1:ncol(test_data)-1)]</pre>
}else{
  stop('No dataset found')
# Create a vector of random seeds for reproducibility
# Note: Boston Housing has more random seeds as its data size is small
if( data_name == 'BostonHousing'){
  seed_vector <- c(1, 1010, 4, 781, 9990, 9999, 81, 46, 67, 2, 3, 1017)
}else{
  seed_vector \leftarrow c(1, 4, 781)
for(i in 1:length(seed_vector)){
  m \leftarrow m + 1
  seed.number <- seed_vector[i]</pre>
```

```
set.seed( seed.number )
 startTime <- Sys.time()</pre>
            <- glinternet.cv(X, Y, numLevels = rep(1, ncol(X)),
                              family = 'gaussian', nFolds = numberCV[j],
                              numCores = 1, verbose = TRUE)
  endTime <- Sys.time()</pre>
  # Obtain main effects and interaction
 coeff <- coef(fit)</pre>
 p_0 <- length(coeff$mainEffects$cat) + length(coeff$mainEffects$cont)</pre>
 p_1 <- length(coeff$interactions$catcat) +</pre>
   length(coeff$interactions$contcat) +
    length(coeff$interactions$contcont)
 k \leftarrow p_0 + p_1
  # calculate RMSE
 prediction <- data.frame(truth = Y, pred = fit$fitted)</pre>
 train_rmse <- mean((prediction$truth-prediction$pred)^2)^0.5</pre>
  # predict on test data
 test_prediction <- data.frame(truth = test_Y, pred = predict(fit, test_X))</pre>
 test rmse <- mean((test prediction $truth-test prediction $pred)^2)^0.5
  # Export the granular info as JSON
 result <- list( colnames = colnames(X),
                  mainEffects = coeff$mainEffects,
                  interactions = coeff$interactions,
                  train_rmse = train_rmse,
                  test_rmse = test_rmse,
                  lambda = fit$lambdaHat,
                  runtime = as.numeric(endTime - startTime ))
 write(toJSON(result, auto_unbox = TRUE, pretty = TRUE, factor = 'string'),
        paste0('glinternet_', data_name, '_', seed.number, '.txt'))
  # Append the all result summary
 all_result[m, 'dataset'] <- data_files[j]</pre>
 all_result[m, 'seed'] <- seed.number</pre>
 all_result[m, 'lambda']
                              <- result$lambda</pre>
 all_result[m, 'p_0']
                              <- p_0
 all_result[m, 'p_1']
 all_result[m, 'train_rmse']<- train_rmse</pre>
 all_result[m, 'test_rmse'] <- test_rmse</pre>
# Save the result summary
write.csv(all_result,
```

```
paste0('glinternet_regr_',data_files[j],'.csv'),
            row.names = FALSE)
}
# 3. Learning interactions using SP-FSR for linear regresssion task ----
for(j in 1:length(data_files)){
  # Initialise the all_result data.frame to store the result
 m <- 0
 results_summary <- data.frame()</pre>
 data_name
              <- data_files[j]</pre>
              <- targets[j]</pre>
 target
  try(
    {
                  <- read.csv(paste0(data_files[j], '_train.csv'))</pre>
      test_data <- read.csv(paste0(data_files[j],'_test.csv'))</pre>
    }
  )
  task <- makeRegrTask(data = data, target = target)</pre>
  # Create a vector of random seeds for reproducibility
  # Note: Boston Housing has more random seeds as its data size is small
  if( data_name == 'BostonHousing'){
    seed_vector <- c(1, 1010, 4, 781, 9990, 9999, 81, 46, 67, 2, 3, 1017)
  }else{
    seed_vector <- c(1, 4, 781)
 for(i in 1:length(seed_vector)){
    seed.number <- seed_vector[i]</pre>
    set.seed(seed.number)
    # Auto feature selection of main effects ----
    spsaMod <- spFeatureSelection( task = task,</pre>
                                     wrapper = wrapper,
                                     measure = mlr::rmse,
                                     num.features.selected = 0,
                                     norm.method = NULL,
                                     cv.stratify = FALSE,
                                     num.cv.folds = numberCV[j])
    # Store the result
    m \leftarrow m + 1
    results_importance
                                   <- list()
    est_coeff
                                   <- list()
    results_summary[m, 'dataset'] <- data_name</pre>
    results_summary[m, 'seed']
                                       <- seed.number
```

```
results_summary[m, 'p_0']
                                    <- length(spsaMod$features)
results_summary[m, 'mean_0']
                                    <- spsaMod$best.value</pre>
results_summary[m, 'std_0']
                                    <- spsaMod$best.std</pre>
results_summary[m, 'runtime_0']
                                    <- spsaMod$run.time</pre>
k <- 1
results_importance[[k]] <- getImportance(spsaMod)</pre>
features.to.keep <- as.character(results importance[[k]]$features)</pre>
                  <- task$task.desc$target</pre>
fittedTask
               <- makeRegrTask(data[, c(features.to.keep, target)],</pre>
                                 target = target, id = 'subset')
               <- train(wrapper, fittedTask)
fittedMod
pred
               <- predict(fittedMod, fittedTask)</pre>
fittedMod
               <- fittedMod$learner.model</pre>
est_coeff[[k]] <- data.frame(coefficient = fittedMod$coefficients)</pre>
# Select interactions ----
sub_task <- modifiedMakeRegrTask(data = data[, c(features.to.keep, target)],</pre>
                                    target = target, order = 2L)
sub_spsaMod <- spFeatureSelection( task = sub_task,</pre>
                                      wrapper = wrapper,
                                      measure = mlr::rmse,
                                      num.features.selected = 0,
                                      norm.method = NULL,
                                      features.to.keep = features.to.keep,
                                      cv.stratify = FALSE,
                                      num.cv.folds = numberCV[j])
k < - k + 1
                                  <- length(sub_spsaMod$features)
results_summary[m, 'p_1']
results_summary[m, 'mean_1']
                                  <- sub_spsaMod$best.value</pre>
results_summary[m, 'std_1']
                                  <- sub_spsaMod$best.std</pre>
results_summary[m, 'runtime_1'] <- sub_spsaMod$run.time
results_importance[[k]]
                                  <- getImportance(sub_spsaMod)</pre>
new features
                <- as.character(results importance[[k]]$features)
sub_fittedtask <- makeRegrTask(sub_task$env$data[, c(new_features, target)],</pre>
                                 target = target, id = 'subset')
sub_fittedMod <- train(wrapper, sub_fittedtask)</pre>
sub_pred
               <- predict(sub_fittedMod, sub_fittedtask)</pre>
est_coeff[[k]] <- data.frame(coefficient = sub_fittedMod$learner.model$coefficients)</pre>
results_summary[m, 'train_AIC']
                                      <- AIC( sub_fittedMod$learner.model)
results_summary[m, 'train_BIC']
                                    <- BIC( sub_fittedMod$learner.model )</pre>
results_summary[m, 'train_rmse']
                                      <- mlr::performance(sub_pred, mlr::rmse)
```

```
# Predict on the test data
    sub_test_task <- modifiedMakeRegrTask(data =</pre>
                                               test_data[, c(features.to.keep, target)],
                                             target = target, order = 2L,
                                             remove.constant = FALSE)
    sub_test_task <- makeRegrTask(data =</pre>
                                      sub test task$env$data[, c(new features, target)],
                                    target = target, id = 'test subset')
    sub_pred_test <- predict(sub_fittedMod, sub_test_task)</pre>
    results_summary[m, 'test_rmse']
                                         <- mlr::performance( sub_pred_test, mlr::rmse)</pre>
    # Prediction w/o interaction terms
                     <- makeRegrTask(data = test_data, target = target)</pre>
    test_pred_noint <- predict(spsaMod$best.model, test_task)</pre>
    train_pred_noint <- predict(spsaMod$best.model, task)</pre>
    results summary[m, 'test rmse']
                                            <- mlr::performance( sub_pred_test, mlr::rmse)</pre>
    results_summary[m, 'test_rmse_noint'] <- mlr::performance(test_pred_noint, mlr::rmse)</pre>
    results_summary[m, 'train_rmse_noint'] <- mlr::performance(train_pred_noint, mlr::rmse)
    final_result <- list(features = new_features,</pre>
                            est_coeff = est_coeff,
                            results_importance,
                            result = results_summary[m, ])
    write(toJSON(final_result, auto_unbox = TRUE, pretty = TRUE, factor = 'string'),
          paste0('spfsr_',data_name,'_',seed.number,'.txt'))
  }
  write.csv(results_summary,
            paste0('spfsr_regr_',data_files[j],'.csv'),
            row.names = FALSE)
}
# 4. Learning interactions using GA for linear regresssion task ----
# Define GA control
GActrl <- makeFeatSelControlGA(maxit = 100)</pre>
for(j in 1:length(data_files)){
  # Initialise the all_result data.frame to store the result
  m < -0
 results_summary <- data.frame()
 data_name <- data_files[j]</pre>
  try(
   {
                  <- read.csv(paste0(data_files[j], '_train.csv'))</pre>
      test_data
                  <- read.csv(paste0(data_files[j],'_test.csv'))</pre>
    }
  )
```

```
task <- makeRegrTask(data = data, target = targets[j])</pre>
# Create a vector of random seeds for reproducibility
# Note: Boston Housing has more random seeds as its data size is small
if( data_name == 'BostonHousing'){
  seed_vector <- c(1, 1010, 4, 781, 9990, 9999, 81, 46, 67, 2, 3, 1017)
}else{
 seed_vector \leftarrow c(1, 4, 781)
for(i in 1:length(seed_vector)){
  seed.number <- seed_vector[i]</pre>
 set.seed(seed.number)
 m \leftarrow m + 1
  # Resampling
              <- makeResampleDesc(method = 'CV' , iters = numberCV[j])</pre>
  # Extract main effects
 main_sfeats <- selectFeatures(wrapper, task = task, resampling = rdesc,</pre>
                                 control = GActrl, show.info = TRUE,
                                 measures = mlr::rmse )
  # Obtain the performance with main effects only
 reduced_main_task <- makeRegrTask(id = 'reduced main',</pre>
                                     data = data[, c(main_sfeats$x , targets[j])],
                                     target = targets[j])
  # Add interactions
  second_task <- modifiedMakeRegrTask(id = 'interaction',</pre>
                                         data = data[, c(main_sfeats$x , targets[j])],
                                         target = targets[j], order = 2L)
  second_sfeats <- selectFeatures(wrapper, task = second_task,</pre>
                                   resampling = rdesc,
                                   control = GActrl, show.info = TRUE,
                                   measures = mlr::rmse )
 results_summary[m, 'dataset']
                                      <- data_name
 results_summary[m, 'seed_number'] <- seed.number</pre>
 results_summary[m, 'p_0']
                                      <- length(main_sfeats$x)
  signif_terms
                   <- as.character(unique(c(main_sfeats$x)))</pre>
 results_summary[m, 'p_1'] <- length(signif_terms) - length(main_sfeats$x)
  # Add the omitted main effects
 third_task <- makeRegrTask(id = 'strong hierarchy',</pre>
                              data = second_task$env$data[, c(signif_terms, targets[j])],
                              target = targets[j])
  constrainedMod <- train( wrapper, third_task )</pre>
```

```
constrainedPred <- predict( constrainedMod, third_task)</pre>
 results_summary[m, 'train_rmse'] <- performance( constrainedPred , measure = mlr::rmse)
 results_summary[m, 'train_AIC'] <- AIC( constrainedMod$learner.model)</pre>
 results_summary[m, 'train_BIC'] <- BIC( constrainedMod$learner.model)</pre>
  sub test task <- modifiedMakeRegrTask(data = test data, target = targets[j],</pre>
                                          order = 2L, remove.constant = FALSE)
  sub_test_task <- makeRegrTask(sub_test_task$env$data[, c(signif_terms, targets[j])],</pre>
                                  target = targets[j], id = 'test_subset')
                         <- predict(constrainedMod , sub_test_task)</pre>
  sub_pred_test
 results_summary[m, 'test_rmse'] <- performance( sub_pred_test, measure = mlr::rmse)
 output <- list(coeff = constrainedMod$learner.model$coefficients,</pre>
                 result = results_summary[m, ],
                 features = signif_terms)
 write(toJSON(output, auto_unbox = TRUE, pretty = TRUE, factor = 'string'),
        paste0('GA_',data_name,'_',seed.number,'.txt'))
}
write.csv(results_summary,
          paste0('GA_regr_',data_files[j],'.csv'),
          row.names = FALSE)
```

R. Codes for Classification Tasks

Baseline Learner for Classification

```
# 2. Loop for each dataset ----
for(j in 1:length(data_files) ){
  train_data <- read.csv(paste0(data_files[j], '_train.csv'))</pre>
  test_data <- read.csv(paste0(data_files[j],'_test.csv'))</pre>
  train_task <- makeClassifTask(data = train_data, target = targets[j])</pre>
  test_task <- makeClassifTask(data = test_data, target = targets[j])</pre>
  baseModel <- train(wrapper, train_task)</pre>
  train_pred <- predict(baseModel, train_task)</pre>
  test_pred <- predict(baseModel, test_task)</pre>
  result[j, 'Data'] <- data_files[j]</pre>
  result[j, 'AIC'] <- AIC(baseModel$learner.model)</pre>
  result[j, 'BIC'] <- BIC(baseModel$learner.model)</pre>
  result[j, 'Train_logLoss'] <- mlr::performance(train_pred, mlr::logloss)
  result[j, 'Test_logLoss'] <- mlr::performance(test_pred, mlr::logloss)</pre>
 result[j, 'Train_auc'] <- mlr::performance(train_pred, mlr::auc)
result[j, 'Test_auc'] <- mlr::performance(test_pred, mlr::auc)</pre>
}
# Save the result as a csv file
write.csv(result, 'baselearner_classif.csv', row.names = FALSE)
```

Modified Make Classification Task Function

```
#' Odescription Generating pairwise interaction terms of a data
#'
                 and pass in to a task
#' Oparam data A data frame containing the features and target variable(s)
#' Oparam target Name of the target variable
#' Cparam order Interaction order. The allowed values are 1, 2, and 3.
# '
               Default is 2L
modifiedMakeClassifTask <- function(data, target, order = 2,</pre>
                                    remove.constant = FALSE,...){
  # Argument check on "order"
  # It is not necessary to check on "data" or "target" as they will
  # be handled by makeClassifTask function
  if( !order %in% c(1, 2, 3) | !inherits(order, 'integer')){
    stop('order must be 1, 2, or 3.')
  # create the classification task
         <- mlr::makeClassifTask(data = data, target = target, ...)</pre>
  task
  if( order %in% c(2, 3)){
    # extract target and descriptive features
   y <- task\env\data[, target]
```

```
if( order == 2){
      fml <- formula(paste0(target, "~.*."))</pre>
    }else{
      fml <- formula(paste0(target, "~.^3"))</pre>
    }
        <- data.frame(model.matrix(fml, task$env$data))
    # Remove constant terms
    if(remove.constant){
      X <- mlr::removeConstantFeatures(X)</pre>
    # bind the data
    newdata <- cbind(X,y)</pre>
    colnames(newdata)[ncol(newdata)] <- target</pre>
    # prompt warning message if p > n
    p \leftarrow ncol(X)
    if( p > nrow(X)){
      warning('More features than number of observations.')
    # reconfigure the task
    task <- mlr::makeClassifTask(data = newdata, target = target, ...)</pre>
  }
  return(task)
}
```

Automatic Feature Selection Script for Classification Tasks

```
# O. Preliminary ----
# Load the relevant packages
library(mlr)
library(spFSR)
library(jsonlite)
library(glinternet)
library(pROC)
library(MASS)
library(ROCR)
source('modifiedMakeClassifTask.R')
# Create a vector of random seeds for reproducibilty
seed_vector <- c(1, 1010, 4, 781, 9990, 9999, 81, 46, 67, 2, 3, 1017)
measure
          <- mlr::auc
# Configuration of common task, wrapper and control
wrapper <- makeLearner('classif.logreg', predict.type = 'prob')</pre>
rdesc <- makeResampleDesc(method = 'CV', stratify = TRUE, iters = 5)</pre>
# 1. Learning interactions with SFFS ----
```

```
<- makeFeatSelControlSequential(method = 'sffs',</pre>
ctrl
                                             alpha = 0.001,
                                             beta = 0.0005)
m <- 0
result
        <- data.frame()
datasets <- c('ionosphere', 'Sonar')</pre>
for( j in 1:length(datasets)){
  data_name <- datasets[j]</pre>
  if( data_name == 'ionosphere'){
               <- read.csv('ionosphere_train.csv')</pre>
    data
    target
               <- 'class'
    test_data <- read.csv('ionosphere_test.csv')</pre>
  }else if( data_name == 'Sonar'){
               <- read.csv('Sonar_train.csv')</pre>
    data
               <- 'Class'
    target
    test_data <- read.csv('Sonar_test.csv')</pre>
  }else{
    stop('No dataset found')
  data <- removeConstantFeatures(data)</pre>
  data <- na.omit(data)</pre>
  test_data <- removeConstantFeatures(test_data)</pre>
           <- makeClassifTask(data = data, target = target)</pre>
  for(i in 1:length(seed_vector)){
    seed.number <- seed_vector[i]</pre>
    set.seed(seed.number)
    m \leftarrow m + 1
    # Extract main effects
    main_sfeats <- selectFeatures(wrapper, task = task, resampling = rdesc,</pre>
                                       control = ctrl, show.info = TRUE, measures = measure )
    # Obtain the performance with main effects only
    reduced_main_task <- makeClassifTask(id = 'reduced main',</pre>
                                            data = data[, c(main_sfeats$x , target)],
                                             target = target)
    # Add interactions
    second_task <- modifiedMakeClassifTask(id = 'interaction',</pre>
```

```
data = data[, c(main_sfeats$x , target)],
                                             target = target, order = 2L)
    second_sfeats <- selectFeatures(wrapper, task = second_task, resampling = rdesc,</pre>
                                      control = ctrl, show.info = TRUE, measures = measure )
    result[m, 'dataset']
                               <- data_name
    result[m, 'seed number'] <- seed.number</pre>
    result[m, 'p 0']
                               <- length(main sfeats$x)
    signif_terms <- as.character(unique(c(main_sfeats$x , second_sfeats$x)))</pre>
    result[m, 'p_1'] <- length(signif_terms) - length(main_sfeats$x)</pre>
    # Add the omitted main effects
    third_task <- makeClassifTask( id = 'strong hierarchy',</pre>
                                     data = second_task$env$data[, c(signif_terms, target)],
                                     target = target)
    constrainedMod
                     <- train( wrapper, third_task )</pre>
    constrainedPred <- predict( constrainedMod, third_task)</pre>
    result[m, 'train_auc'] <- performance( constrainedPred , measure = measure)</pre>
    result[m, 'train_AIC'] <- AIC( constrainedMod$learner.model)</pre>
    result[m, 'train BIC'] <- BIC( constrainedMod$learner.model)</pre>
    sub_test_task <- modifiedMakeClassifTask(data = test_data, target = target, order = 2L)</pre>
    sub_test_task <- makeClassifTask(sub_test_task$env$data[, c(signif_terms, target)],</pre>
                                        target = target, id = 'test_subset')
    sub_pred_test
                           <- predict(constrainedMod , sub_test_task)</pre>
    result[m, 'test_auc'] <- performance( sub_pred_test, measure)</pre>
    output <- list(coeff = constrainedMod$learner.model$coefficients,</pre>
                    result = result[m, ],
                    features = signif_terms)
    write(toJSON(output, auto_unbox = TRUE, pretty = TRUE, factor = 'string'),
          paste0('SFFS_',data_name,'_',seed.number,'.txt'))
  }
}
write.csv(result, 'SFFS_results.csv', row.names = FALSE)
# 2. Learning interactions with two-step SP-FSR ----
# Reset the results summary
m <- 0
results_summary <- data.frame()</pre>
```

```
for(j in 1:length(datasets)){
  data_name <- datasets[j]</pre>
  if( data_name == 'ionosphere'){
    data
              <- read.csv('ionosphere_train.csv')</pre>
              <- 'class'
    test_data <- read.csv('ionosphere_test.csv')</pre>
    data <- removeConstantFeatures(data)</pre>
    test_data <- removeConstantFeatures(test_data)</pre>
  }else if( data_name == 'Sonar'){
               <- read.csv('Sonar_train.csv')</pre>
    data
              <- 'Class'
    target
    test_data <- read.csv('Sonar_test.csv')</pre>
    data <- removeConstantFeatures(data)</pre>
    test_data <- removeConstantFeatures(test_data)</pre>
  }else{
    stop('No dataset found')
  task
             <- makeClassifTask(data = data, target = target)</pre>
  for(i in 1:length(seed_vector)){
    seed.number <- seed_vector[i]</pre>
    set.seed(seed.number)
    # Auto feature selection of main effects ----
    spsaMod <- spFeatureSelection( task = task,</pre>
                                      wrapper = wrapper,
                                      measure = measure,
                                      num.features.selected = 0,
                                      norm.method = NULL)
    # Store the result
    m \leftarrow m + 1
    results_importance
                                  <- list()
                                    <- list()
    est_coeff
    results_summary[m, 'dataset']
                                        <- data_name
    results_summary[m, 'seed']
                                        <- seed.number
    results_summary[m, 'p_0']
                                        <- length(spsaMod$features)</pre>
    results_summary[m, 'mean_0']
                                        <- spsaMod$best.value</pre>
    results_summary[m, 'std_0']
                                        <- spsaMod$best.std</pre>
    results_summary[m, 'runtime_0']
                                        <- spsaMod$run.time</pre>
    k <- 1
    results_importance[[k]] <- getImportance(spsaMod)</pre>
```

```
features.to.keep <- as.character(results_importance[[k]]$features)</pre>
                 <- task$task.desc$target</pre>
target
fittedTask
              <- makeClassifTask(data[, c(features.to.keep, target)],</pre>
                                   target = target, id = 'subset')
fittedMod
             <- train(wrapper, fittedTask)</pre>
pred
               <- predict(fittedMod, fittedTask)</pre>
fittedMod
               <- fittedMod$learner.model</pre>
est coeff[[k]] <- data.frame(coefficient = fittedMod$coefficients)</pre>
# Select interactions ----
sub_task <- modifiedMakeClassifTask(data = data[, c(features.to.keep, target)],</pre>
                                     target = target, order = 2L)
sub_spsaMod <- spFeatureSelection( task = sub_task,</pre>
                                    wrapper = wrapper,
                                    measure = measure,
                                    num.features.selected = 0,
                                     norm.method = NULL,
                                     features.to.keep = features.to.keep)
k \leftarrow k + 1
results_summary[m, 'p_1']
                                <- length(sub spsaMod$features)
results_summary[m, 'mean_1'] <- sub_spsaMod$best.value</pre>
results summary[m, 'std 1'] <- sub spsaMod$best.std
results_summary[m, 'runtime_1'] <- sub_spsaMod$run.time</pre>
results_importance[[k]]
                                <- getImportance(sub_spsaMod)</pre>
new_features <- as.character(results_importance[[k]]$features)</pre>
sub_fittedtask <- makeClassifTask(sub_task$env$data[, c(new_features, target)],</pre>
                                   target = target, id = 'subset')
sub_fittedMod <- train(wrapper, sub_fittedtask)</pre>
sub_pred
              <- predict(sub_fittedMod, sub_fittedtask)</pre>
est_coeff[[k]] <- data.frame(coefficient = sub_fittedMod$learner.model$coefficients)</pre>
results_summary[m, 'train_logloss'] <- mlr::performance(sub_pred, mlr::logloss)
# Predict on the test data
sub_test_task <- modifiedMakeClassifTask(data =</pre>
                                             test_data[, c(features.to.keep, target)],
                                           target = target, order = 2L)
sub_test_task <- makeClassifTask(sub_test_task$env$data[, c(new_features, target)],</pre>
                                   target = target, id = 'test_subset')
sub_pred_test <- predict(sub_fittedMod, sub_test_task)</pre>
```

```
results_summary[m, 'test_auc'] <- mlr::performance( sub_pred_test, measure)</pre>
    results_summary[m, 'test_logloss'] <- mlr::performance( sub_pred_test, mlr::logloss)</pre>
    # Prediction w/o interaction terms
    test_task <- makeClassifTask(data = test_data, target = target)</pre>
    test_pred_noint <- predict(spsaMod$best.model, test_task)</pre>
    train_pred_noint <- predict(spsaMod$best.model, task)</pre>
    results summary[m, 'test auc']
                                     <- mlr::performance( sub_pred_test, measure)</pre>
    results_summary[m, 'test_logloss'] <- mlr::performance( sub_pred_test, mlr::logloss)
    results_summary[m, 'test_auc_noint'] <- mlr::performance(test_pred_noint,
                                                                   mlr::auc)
    results_summary[m, 'test_logloss_noint'] <- mlr::performance(test_pred_noint,
                                                                   mlr::logloss)
    results_summary[m, 'train_auc_noint'] <- mlr::performance(train_pred_noint,
                                                                    mlr::auc)
    results_summary[m, 'train_logloss_noint'] <- mlr::performance(train_pred_noint,
                                                                    mlr::logloss)
                  <- list(features = new_features,
    final result
                           est_coeff = est_coeff,
                           results_importance,
                           result = results summary[m, ])
    write(toJSON(final_result, auto_unbox = TRUE, pretty = TRUE, factor = 'string'),
          paste0('spfsr_',data_name,'_',seed.number,'.txt'))
  }
}
write.csv(results_summary, 'spfsr_results.csv', row.names = FALSE)
# 3. Learning interactions with glinternet ----
# Reset the data frame
m <- 0
all result <- data.frame()
for(j in 1:length(datasets)){
  data_name <- datasets[j]</pre>
  if( data_name == 'ionosphere'){
    data <- read.csv('ionosphere_train.csv')</pre>
    Y <- ifelse(data$class == 'b', 1, 0)
    data <- removeConstantFeatures(data)</pre>
          <- data[, c(1:ncol(data)-1)]
    test_data <- read.csv('ionosphere_test.csv')</pre>
    test_data <- removeConstantFeatures(test_data)</pre>
           <- ifelse(test_data$class == 'b', 1, 0)
```

```
test_X <- test_data[, c(1:ncol(test_data)-1)]</pre>
}else if( data_name == 'Sonar'){
  data <- read.csv('Sonar_train.csv')</pre>
  Y <- ifelse(data$Class == 'R', 1, 0)
  data <- removeConstantFeatures(data)</pre>
        <- data[, c(1:ncol(data)-1)]
  test_data <- read.csv('Sonar_test.csv')</pre>
  test_data <- removeConstantFeatures(test_data)</pre>
  test Y
          <- ifelse(test_data$Class == 'R', 1, 0)</pre>
            <- test_data[, c(1:ncol(test_data)-1)]</pre>
  test_X
}else{
  stop('No dataset found')
for(i in 1:length(seed_vector)){
  m \leftarrow m + 1
  seed.number <- seed_vector[i]</pre>
  set.seed( seed.number )
  # hierarchical group-lasso regularization (CV = 10)
  startTime <- Sys.time()</pre>
             <- glinternet.cv(X, Y, numLevels = rep(1, ncol(X)),
                               family = 'binomial', nFolds = 5)
  endTime
            <- Sys.time()
  # Obtain main effects and interaction
  coeff <- coef(fit)</pre>
  p_0 <- length(coeff$mainEffects$cat) +</pre>
    length(coeff$mainEffects$cont)
  p_1 <- length(coeff$interactions$catcat) +</pre>
    length(coeff$interactions$contcat) +
    length(coeff$interactions$contcont)
  k \leftarrow p_0 + p_1
  # calculate AIC and BIC
  prediction <- data.frame(truth = Y, pred = fit$fitted)</pre>
             <- sum(prediction$truth*log(prediction$pred) + (1-prediction$truth)*log(1-prediction$pre</pre>
  logLik
  AIC
             <- -2*logLik + 2*k
  BIC
             <- -2*logLik + log(nrow(X))*k
  # predict on test data
  test_prediction <- data.frame(truth = test_Y,</pre>
                                  pred = predict(fit, test_X))
                  <- sum(test_prediction$truth*log(test_prediction$pred) +
  test_logLik
```

```
(1-test_prediction$truth)*log(1-test_prediction$pred))
                    <- -2*test_logLik + 2*k
    {\sf test\_AIC}
    {\sf test\_BIC}
                    <- -2*test_logLik + log(nrow(test_X))*k
    # Store the result
    result <- list( colnames = colnames(X),
                    mainEffects = coeff$mainEffects,
                    interactions = coeff$interactions,
                    train_auc = auc(Y, fit$fitted),
                    AIC = AIC,
                    BIC = BIC,
                    test_auc = auc(test_prediction$truth, test_prediction$pred),
                    test_AIC = test_AIC,
                    test_BIC = test_BIC,
                    train_logloss = -logLik/nrow(data),
                    test_logloss = -test_logLik/nrow(test_data),
                    lambda = fit$lambdaHat,
                    runtime = as.numeric(endTime - startTime ))
    write(toJSON(result, auto_unbox = TRUE, pretty = TRUE, factor = 'string'),
          paste0('glinternet_', data_name, '_', seed.number, '.txt'))
    # Store the all result summary
    all_result[m, 'dataset'] <- datasets[j]</pre>
    all_result[m, 'seed'] <- seed.number</pre>
    all_result[m, 'lambda'] <- result$lambda</pre>
    all_result[m, 'train_auc'] <- result$train_auc</pre>
    all_result[m, 'train_AIC'] <- result$AIC</pre>
    all_result[m, 'train_BIC'] <- result$BIC</pre>
    all_result[m, 'train_logloss'] <- result$train_logloss</pre>
    all_result[m, 'p_0']
                                <- p_0
    all_result[m, 'p_1']
                                <- p_1
    all_result[m, 'test_auc'] <- result$test_auc
    all_result[m, 'test_AIC'] <- result$test_AIC</pre>
    all_result[m, 'test_BIC'] <- result$test_BIC</pre>
    all_result[m, 'test_logloss'] <- result$test_logloss</pre>
 }
}
# Save the result summary
write.csv(all_result, 'glinternet_all_result.csv', row.names = FALSE)
# 4. Learning interactions with GA ----
```

```
result <- data.frame()
         <- makeFeatSelControlGA( maxit = 20)
for( j in 1:length(datasets)){
  data_name <- datasets[j]</pre>
  if( data_name == 'ionosphere'){
               <- read.csv('ionosphere_train.csv')</pre>
    data
    target
               <- 'class'
    test_data <- read.csv('ionosphere_test.csv')</pre>
  }else if( data_name == 'Sonar'){
    data
               <- read.csv('Sonar_train.csv')
    target
              <- 'Class'
    test_data <- read.csv('Sonar_test.csv')</pre>
  }else{
    stop('No dataset found')
  data <- removeConstantFeatures(data)</pre>
  data <- na.omit(data)</pre>
  test_data <- removeConstantFeatures(test_data)</pre>
            <- makeClassifTask(data = data, target = target)</pre>
  for(i in 1:length(seed_vector)){
    seed.number <- seed_vector[i]</pre>
    set.seed(seed.number)
    m \leftarrow m + 1
    # Extract main effects
    main_sfeats <- selectFeatures(wrapper, task = task, resampling = rdesc,</pre>
                                      control = ctrl, show.info = TRUE, measures = measure )
    # Obtain the performance with main effects only
    reduced_main_task <- makeClassifTask(id = 'reduced main',</pre>
                                            data = data[, c(main_sfeats$x , target)],
                                            target = target)
    # Add interactions
    second_task <- modifiedMakeClassifTask(id = 'interaction',</pre>
                                              data = data[, c(main_sfeats$x , target)],
                                              target = target, order = 2L)
    second_sfeats <- selectFeatures(wrapper, task = second_task, resampling = rdesc,</pre>
                                      control = ctrl, show.info = TRUE, measures = measure )
```

```
result[m, 'dataset']
                               <- data name
    result[m, 'seed_number'] <- seed.number</pre>
    result[m, 'p_0']
                               <- length(main_sfeats$x)
    signif_terms <- as.character(unique(c(main_sfeats$x , second_sfeats$x)))</pre>
    result[m, 'p_1'] <- length(signif_terms) - length(main_sfeats$x)</pre>
    # Add the omitted main effects
    third_task <- makeClassifTask( id = 'strong hierarchy',</pre>
                                     data = second_task$env$data[, c(signif_terms, target)],
                                     target = target)
                     <- train( wrapper, third_task )</pre>
    constrainedMod
    constrainedPred <- predict( constrainedMod, third_task)</pre>
    result[m, 'train_auc'] <- performance( constrainedPred , measure = measure)</pre>
    result[m, 'train_AIC'] <- AIC( constrainedMod$learner.model)</pre>
    result[m, 'train_BIC'] <- BIC( constrainedMod$learner.model)</pre>
    sub_test_task <- modifiedMakeClassifTask(data = test_data, target = target, order = 2L)</pre>
    sub_test_task <- makeClassifTask(sub_test_task$env$data[, c(signif_terms, target)],</pre>
                                        target = target, id = 'test_subset')
                           <- predict(constrainedMod , sub_test_task)</pre>
    sub_pred_test
    result[m, 'test_auc'] <- performance( sub_pred_test, measure)</pre>
    output <- list(coeff = constrainedMod$learner.model$coefficients,</pre>
                    result = result[m, ],
                    features = signif_terms)
    write(toJSON(output, auto_unbox = TRUE, pretty = TRUE, factor = 'string'),
          paste0('GA_',data_name,'_',seed.number,'.txt'))
  }
}
write.csv(result, 'GA_result.csv', row.names = FALSE)
```