Statistical Models HW6

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2023-02-28

Question 1.

Implement k-fold cross-validation and sequential model selection for linear regression models.

```
library(MASS)
dat = Boston[, -c(4, 9)]
dat = dat[,c("crim","zn","nox","rm","dis","ptratio","black","lstat","medv")]
x = dat[,!names(dat) %in% c('medv')]
y <- data.frame(medv = dat$medv)
#x <- Boston[, -c(4, 9)]
#y <- Boston[, 14]
```

1a)

Write a function cv.lm(x, y, k) which estimates the prediction error of the linear regression model with y as response using k-fold cross-validation

```
cv.lm <- function(x,y, k) {
  # x is a matrix of predictors
  # y is a vector of response
  # k is the number of folds
  # returns the mean squared error of the model


  #dat_cv = dat[sample(n),]
  n = nrow(x)
  dat_cv = data.frame(x,y)
  dat_cv = dat_cv[sample(n),]
  #print(dat_cv)
  folds <- cut(seq(1,n),breaks=k,labels=FALSE)
  cv_error = rep(NA, k)

  # construct formula string
  formula_string <- paste(paste(colnames(y), collapse = " + "),
                          " ~", paste(colnames(x), collapse = " + "))
  # convert formula string to formula object
  formula_object <- as.formula(formula_string)

  #k is the number of folds
  for (i in 1:k)
```

```r
  {
    #Creating train and validation subsets from folds
    dat_train = dat_cv[folds != i,]
    dat_val = dat_cv[folds == i,]

    #training model
    train_model = lm(formula_object, data = dat_train)
    #train_model = lm(medv ~ crim + zn + nox + rm + dis + ptratio + black + lstat, data = dat_train)
    pred_val = predict(train_model, newdata = dat_val)

    #Calculating cross validation error at ith fold
    cv_error[i] = sqrt(mean((dat_val$medv - pred_val)^2))
   }

  #return mean of CV error
  return(mean(cv_error))
}
```

```r
#Testing on the Boston dataset
cv.lm(x, y, 5)
```

```
## [1] 4.881043
```

```r
#Using caret
library(caret)
cv.lm_with_caret <- function(x, y, k) {
  # x is a matrix of predictors
  # y is a vector of response
  # k is the number of folds
  # returns the mean squared error of the model
  n = nrow(x)
  dat_cv = data.frame(x,y)

  train_control <- trainControl(method = "cv",number = k)
  m_cv <- train(medv ~ ., data = dat_cv,
                method = "lm",
                trControl = train_control)

  print(m_cv)
  rmse <- m_cv$results$RMSE[length(m_cv$results$RMSE)]
  return(rmse)
}

cv.lm_with_caret(x, y, 5)
```

```
## Linear Regression
##
## 506 samples
##   8 predictor
##
## No pre-processing
## Resampling: Cross-Validated (5 fold)
```

```
## Summary of sample sizes: 405, 405, 404, 406, 404
## Resampling results:
##
##   RMSE      Rsquared  MAE
##   4.953714  0.711479  3.407244
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

```
## [1] 4.953714
```

Inference:

As we can see above, the cv.lm(x,y,k) function which calculates the k -fold cross validation root mean squared error stepwise and the cv.lm_with_caret(x,y,k) function which uses pre built library function to calculate the k -fold cross validation root mean squared error. We test our own function with the Boston data set selecting the required variables and giving k-folds. We observe that both the functions give almost same value that is 4.9, which validates the correctness of our function.

1b

Write a function SequentialSelection(x, y, method) which computes the forward selection path for linear regression from 'intercept only' to 'full model' and chooses the model on that path using different criteria specified by method. The function should support these methods:

- method = "AdjR2": Sequentially include the columns of x and choose the model that gives the largest adjusted R2.
- method = "AIC": Sequentially include the columns of x and choose the model that gives the smallest AIC.
- method = "CV5": Sequentially include the columns of x and choose the model that gives the smallest 5-fold cross-validation prediction error.

```
dat = Boston[, -c(4, 9)]
dat = dat[,c("crim","zn","nox","rm","dis","ptratio","black","lstat","medv")]
x = dat[,!names(dat) %in% c('medv')]
y = dat$medv
```

#new code

```
SequentialSelection <- function(x, y, method) {
  # x is the design matrix
  # y is the response variable
  # method is a string indicating the selection criteria

  # initialize variables
  p <- ncol(x)
  n <- nrow(x)
  included <- c() # columns included in the model
  #excluded <- 1:p # columns excluded from the model
  cols = c(colnames(x))
  excluded <- c(colnames(x)) # columns excluded from the model
```

```r
#print("formula_object")
#print(cols)

intercept <- rep(1, n) # intercept only model
models <- list(intercept)
scores <- c()

if(method == "ADJR2"){

  # loop over columns
  for (i in 1:p) {
    best_score <- NULL
    best_col <- NULL

    # loop over excluded columns
    for (j in excluded) {

      # fit model with j-th column included
      features = c(included, j)

      # construct formula string
      formula_string <- paste("y ~", paste(features, collapse = " + "))

      # convert formula string to formula object
      formula_object <- as.formula(formula_string)


      #model <- lm(y ~ x[, c(included, j)])
      # fit model with features from list
      #print("formula_object")
      #print(formula_object)
      model <- lm(formula_object, data = x)
      score <- summary(model)$adj.r.squared

      # update best score and column
      if (is.null(best_score) || score > best_score) {
        best_score <- score
        best_col <- j
      }
    }

    # add best column to included columns and remove from excluded columns
    included <- c(included, best_col)
    excluded <- setdiff(excluded, best_col)

    ## saving the best model
    formula_string <- paste("y ~", paste(included, collapse = " + "))
    formula_object <- as.formula(formula_string)
    models[i] <- lm(formula_object, data = x)
    scores[i] <- best_score
  }
}
else {
```

```r
  #print("inside else")
  # loop over columns
  for (i in 1:p) {
    best_score <- NULL
    best_col <- NULL

    # loop over excluded columns
    for (j in excluded) {

      # fit model with j-th column included
      features = c(included, j)

      # construct formula string
      formula_string <- paste("y ~", paste(features, collapse = " + "))

      # convert formula string to formula object
      formula_object <- as.formula(formula_string)


      #model <- lm(y ~ x[, c(included, j)])
      # fit model with features from list
      #print("formula_object")
      #print(formula_object)
      model <- lm(formula_object, data = x)


      # compute score based on method

      if (method == "AIC") {
        score <- AIC(model)
      } else if (method == "CV5") {
        score <- mean(sapply(split(1:n, rep(1:5, each = n/5)), function(ind){
          mean((y[ind] - predict(model, newdata = x[ind,]))^2)
        }))
      } else {
        stop("Invalid method")
      }

      # update best score and column
      if (is.null(best_score) || score < best_score) {
        best_score <- score
        best_col <- j
      }
    }

    # add best column to included columns and remove from excluded columns
    included <- c(included, best_col)
    excluded <- setdiff(excluded, best_col)

    ## saving the best model
    formula_string <- paste("y ~", paste(included, collapse = " + "))
    formula_object <- as.formula(formula_string)
    models[i] <- lm(formula_object, data = x)
```

```r
      scores[i] <- best_score
    }
  }


  #print("scores")
  #print(scores)
  #print("models")
  #print(models)
  #print("models end")

  # choose best model based on method


  if (method == "ADJR2") {
    best_model <- models[[which.max(scores)]]
  } else if (method == "AIC") {
    best_model <- models[[which.min(scores)]]
  } else if (method == "CV5") {
    best_model <- models[[which.min(scores)]]
  } else {
    stop("Invalid method")
  }

  best_score = 0
  # return results
  if (method == "ADJR2"){
    best_score = max(scores)
  }
  else{
    best_score = min(scores)
  }

  print("Best Score")
  print(best_score)

  return(list(included = included, best_model = best_model, best_score = best_score))
}
```

```r
mod = SequentialSelection(x,y, "ADJR2" )
```

```
## [1] "Best Score"
## [1] 0.7176965
```

```r
mod
```

```
## $included
## [1] "lstat"   "rm"      "ptratio" "dis"     "nox"     "black"   "zn"
## [8] "crim"
##
## $best_model
##   (Intercept)         lstat            rm       ptratio           dis
```

```
##  29.549705433  -0.531633914   4.217413502  -0.875832606  -1.463800087
##           nox         black            zn          crim
## -15.213643701   0.008783782   0.041267442  -0.066091682
##
## $best_score
## [1] 0.7176965
```

```r
mod$best_model[]
```

```
##   (Intercept)         lstat            rm       ptratio           dis
##  29.549705433  -0.531633914   4.217413502  -0.875832606  -1.463800087
##           nox         black            zn          crim
## -15.213643701   0.008783782   0.041267442  -0.066091682
```

```r
mod = SequentialSelection(x,y, "AIC" )
```

```
## [1] "Best Score"
## [1] 3052.425
```

```r
mod
```

```
## $included
## [1] "lstat"   "rm"      "ptratio" "dis"     "nox"     "black"   "zn"
## [8] "crim"
##
## $best_model
##   (Intercept)         lstat            rm       ptratio           dis
##  29.549705433  -0.531633914   4.217413502  -0.875832606  -1.463800087
##           nox         black            zn          crim
## -15.213643701   0.008783782   0.041267442  -0.066091682
##
## $best_score
## [1] 3052.425
```

```r
mod$best_model[]
```

```
##   (Intercept)         lstat            rm       ptratio           dis
##  29.549705433  -0.531633914   4.217413502  -0.875832606  -1.463800087
##           nox         black            zn          crim
## -15.213643701   0.008783782   0.041267442  -0.066091682
```

```r
mod = SequentialSelection(x,y, "CV5" )
```

```
## [1] "Best Score"
## [1] 23.4771
```

```r
mod
```

```
## $included
## [1] "lstat"   "rm"      "ptratio" "dis"     "nox"     "black"   "zn"
## [8] "crim"
##
## $best_model
##   (Intercept)         lstat            rm       ptratio           dis
##  29.549705433  -0.531633914   4.217413502  -0.875832606  -1.463800087
##           nox         black            zn          crim
## -15.213643701   0.008783782   0.041267442  -0.066091682
##
## $best_score
## [1] 23.4771
```

```
mod$best_model[]
```

```
##   (Intercept)         lstat            rm       ptratio           dis
##  29.549705433  -0.531633914   4.217413502  -0.875832606  -1.463800087
##           nox         black            zn          crim
## -15.213643701   0.008783782   0.041267442  -0.066091682
```

Inference

We see from the sequential method selection above that for all the 3 methods, AdjR2, CV5 and AIC it gives the best model from the selection. We can see from the values also that it performs reasonable well.

Question2

Consider a regression setting where the predictor variable is real valued and the goal is to fit a polynomial model. Specifically, we assume that x1,. . . ,xn are iid uniform in [0, 2pi] and conditional on these, y1, . . . , yn are independent, with yi normal with mean sin(3xi) + xi and variance 1. Take n = 200 and set the maximum degree at 20. Perform simulations (at least 100 data instances) to compare the choice of degree by the sequential model selection methods in Problem 1. Produce plots of 3 example data instances and their best model fits according to different methods. Produce plots of the distribution of the polynomial degrees chosen by the different methods over all simulated instances. Offer comments on what you observe.

```
data_generation <-function(degree = 20){
  n = 200
  x <- runif(n, 0, 2*pi)
  y <- rnorm(n, mean = sin(3*x) + x, sd = 1)
  return (list(x=x,y=y))
}

data = data_generation()
x = data$x
y= data$y

x = list(x,x^2)
names(x)<- c("x", paste0("x^", 2))

typeof(x)
```

```
## [1] "list"
```

```r
colnames(x)
```

```
## NULL
```

```r
x <- data.frame(x)
colnames(x)
```

```
## [1] "x"   "x.2"
```

```r
SequentialSelection(x,y, method = "CV5")
```

```
## [1] "Best Score"
## [1] 1.44116
```

```
## $included
## [1] "x"   "x.2"
##
## $best_model
## (Intercept)           x         x.2
##  0.77535180  0.48300193  0.06464175
##
## $best_score
## [1] 1.44116
```

```r
max_degree = 20
methods = c("ADJR2", "AIC", "CV5")


adj_deg =  rep(0, 100)
aic_deg =  rep(0, 100)
cv_deg =  rep(0, 100)


x_ =c()
```

```r
#Knitting till 100 took a lot of time so we computed for less
for(i in 1:1){
  data = data_generation()
  x_ = data$x
  y_= data$y
  X <- matrix(rep(x_, 20), ncol = 20)

  for (i in 2:20) {
    X[,i] <- X[,i-1] * x_
    # Create a data frame with the matrix and set column names
    x <- data.frame(X)
    names(x) <- paste0("x", 1:20)
```

```
  for (method in methods){
    best_score = NULL
    best_deg = NULL

    for (deg in 2:max_degree){
      #x = list(x_,x_^deg)
      #names(x)<- c("x", paste0("x^", 2))
      #x <- data.frame(x)
      #result = SequentialSelection(x,y, method = method)
      result = SequentialSelection(x[,1:deg],y, method = method)
      if (method == "ADJR2"){
        best_score = max(best_score, result$best_score)
        best_deg = deg
      }
      else{
        best_score = min(best_score, result$best_score)
        best_deg = deg
      }
    }
    if (method == "ADJR2") {
      adj_deg[i] <- best_deg
    } else if (method == "AIC") {
      aic_deg[i] <- best_deg
    } else if (method == "CV5") {
      cv_deg[i] <- best_deg
    } else {
      stop("Invalid method")
    }
  }
    print(adj_deg[i])
    print(aic_deg[i])
    print(cv_deg)
}
}
```

```
## [1] "Best Score"
## [1] 0.01319954
## [1] "Best Score"
## [1] 0.01319954
## [1] "Best Score"
## [1] 0.01319954
## [1] "Best Score"
## [1] 0.01319954
## [1] "Best Score"
## [1] 0.01319954
## [1] "Best Score"
## [1] 0.01319954
## [1] "Best Score"
## [1] 0.01319954
## [1] "Best Score"
## [1] 0.01319954
## [1] "Best Score"
## [1] 0.01319954
```

```
## [1] "Best Score"
## [1] 0.01319954
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## [1] 0.01319954
## [1] "Best Score"
## [1] 854.6139
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```

```
## [1] "Best Score"
## [1] 854.6139
## [1] "Best Score"
## [1] 854.6139
## [1] "Best Score"
## [1] 4.068927
## [1] "Best Score"
## [1] 4.068927
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## [1] "Best Score"
## [1] 4.068927
## [1] 20
## [1] 20
##   [1]  0 20  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
##  [26]  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
##  [51]  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
##  [76]  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
## [1] "Best Score"
## [1] 0.01319954
## [1] "Best Score"
## [1] 0.01628026
## [1] "Best Score"
## [1] 0.01628026
```

```
## [1] "Best Score"
## [1] 0.01628026
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```

```
## [1] "Best Score"
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## [1] "Best Score"
## [1] 4.068927
## [1] "Best Score"
## [1] 4.023461
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```

```
## [1] 20
## [1] 20
##   [1]  0 20 20  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
##  [26]  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
##  [51]  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
##  [76]  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
## [1] "Best Score"
## [1] 0.01319954
## [1] "Best Score"
## [1] 0.01628026
## [1] "Best Score"
## [1] 0.01865056
## [1] "Best Score"
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## [1] "Best Score"
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## [1] "Best Score"
## [1] 0.01865056
## [1] "Best Score"
## [1] 0.02026872
## [1] "Best Score"
## [1] 0.02123133
## [1] "Best Score"
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## [1] "Best Score"
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## [1] "Best Score"
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## [1] "Best Score"
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## [1] "Best Score"
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## [1] "Best Score"
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## [1] "Best Score"
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## [1] "Best Score"
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Team Contributions

In this HW, both the team members Sourabh Prakash and Priyanshi Shah have contributed equally to the homework by discussing the key points and logic together and doing pair programming. For the implementation part question 1 was contributed by Priyanshi Shah and question 2 by Sourabh Prakash. The inferences were drawn together by both the team members.