# DS-6030 Homework Module 5

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#### DS 6030 | Spring 2023 | University of Virginia

- 8. In this exercise, we will generate simulated data, and will then use this data to perform best subset selection.
  - (a) Use the rnorm() function to generate a predictor X of length n = 100, as well as a noise vector  $\epsilon$  of length n = 100.

```
set.seed(2)
X <- rnorm(n = 100, mean = 0, sd = 1)
epsilon <- rnorm(n = 100, mean = 0, sd = 1*10^{-6})
X[1:3]</pre>
```

**#** [1] -0.8969145 0.1848492 1.5878453

```
epsilon[1:3]
```

- # [1] 1.074459e-06 2.605978e-07 -3.142720e-07
- (b) Generate a response vector Y of length n = 100 according to the model  $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \epsilon$ , where  $\beta_0$ ,  $\beta_1$ ,  $\beta_2$ ,  $\beta_3$  are constants of your choice.

```
beta_0 <- 1
beta_1 <- 2
beta_2 <- 3
beta_3 <- 4
Y <- beta_0 + beta_1 * X + beta_2 * I(X^2) + beta_3 * I(X^3) + epsilon
Y[1:3]</pre>
```

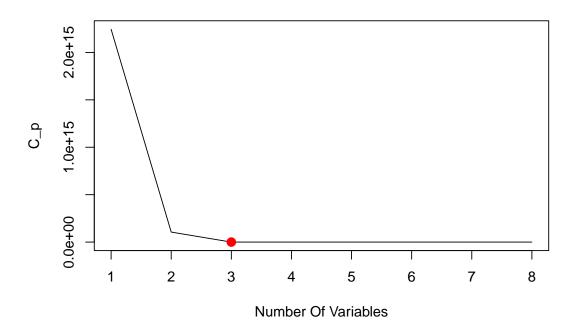
- # [1] -1.266573 1.497471 27.752887
- (c) Use the regsubsets() function to perform best subset selection in order to choose the best model containing the predictors  $X, X^2 \dots, X^{10}$ . What is the best model obtained according to Cp, BIC, and adjusted  $R^2$ ? Show some plots to provide evidence for your answer, and report the coefficients of the best model obtained. Note you will need to use the data.frame() function to create a single data set containing both X and Y.

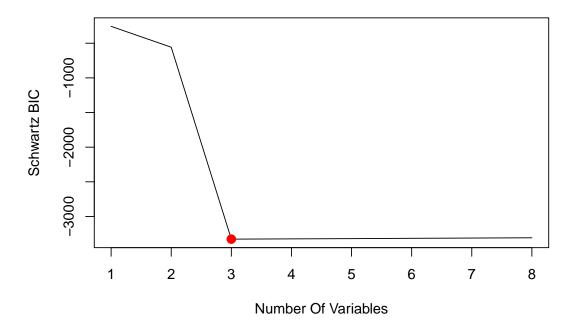
```
data_frame <- data.frame(X = X, Y = Y)
head(data_frame, n = 3)</pre>
```

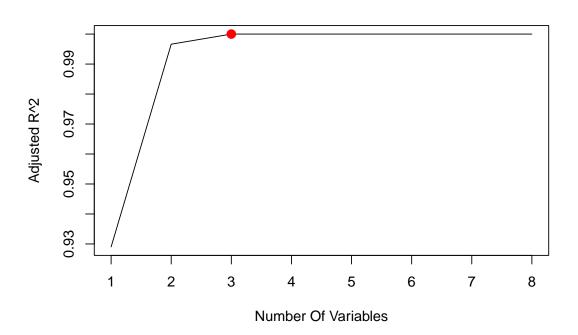
```
# X Y
# 1 -0.8969145 -1.26657....
# 2 0.1848492 1.497470....
# 3 1.5878453 27.75288....
```

```
library(leaps)
formula \leftarrow Y \sim X + I(X^2) + I(X^3) + I(X^4) + I(X^5) + I(X^6) + I(X^7) + I(X^8) + I(X^9) + I(X
subset_selection_object <- regsubsets(</pre>
    x = formula,
    data = data_frame,
    method = "exhaustive"
analyze subset selection object <- function(subset selection object) {
summary_for_subset_selection_object <- summary(object = subset_selection_object)</pre>
Mallows_Cp <- summary_for_subset_selection_object$cp</pre>
index_of_model_with_minimum_Mallows_Cp <- which.min(Mallows_Cp)</pre>
coefficients_by_Mallows_Cp <- coef(</pre>
     subset selection object, index of model with minimum Mallows Cp
)
Schwartz_BIC <- summary_for_subset_selection_object$bic</pre>
 index_of_model_with_minimum_Schwartz_BIC <- which.min(Schwartz_BIC)</pre>
 coefficients_by_Schwartz_BIC <- coef(</pre>
     subset_selection_object, index_of_model_with_minimum_Schwartz_BIC
adjusted_R2 <- summary_for_subset_selection_object$adjr2</pre>
 index_of_model_with_maximum_adjusted_R2 <- which.max(adjusted_R2)
 coefficients_by_adjusted_R2 <- coef(</pre>
     subset_selection_object, index_of_model_with_maximum_adjusted_R2
)
plot(Mallows Cp, xlab = "Number Of Variables", ylab = "C p", type = "1")
 index_of_minimum_Mallows_Cp <- which.min(Mallows_Cp)</pre>
minimum Mallows Cp <- Mallows Cp[index of minimum Mallows Cp]
points(
     index_of_minimum_Mallows_Cp,
     minimum_Mallows_Cp,
     col = "red",
     cex = 2,
     pch = 20
 )
plot(Schwartz_BIC, xlab = "Number Of Variables", ylab = "Schwartz BIC", type = "l")
 index_of_minimum_Schwartz_BIC <- which.min(Schwartz_BIC)</pre>
minimum_Schwartz_BIC <- Schwartz_BIC[index_of_minimum_Schwartz_BIC]
points(
     index_of_minimum_Schwartz_BIC,
     minimum_Schwartz_BIC,
     col = "red",
     cex = 2,
     pch = 20
plot(adjusted_R2, xlab = "Number Of Variables", ylab = "Adjusted R^2", type = "1")
index_of_maximum_adjusted_R2 <- which.max(adjusted_R2)</pre>
maximum_adjusted_R2 <- adjusted_R2[index_of_maximum_adjusted_R2]</pre>
points(
     index_of_maximum_adjusted_R2,
     maximum_adjusted_R2,
     col = "red",
     cex = 2,
     pch = 20
```

```
coefficients <- list(
    coefficients_by_Mallows_Cp = coefficients_by_Mallows_Cp,
    coefficients_by_Schwartz_BIC = coefficients_by_Schwartz_BIC,
    coefficients_by_adjusted_R2 = coefficients_by_adjusted_R2
)
return(coefficients)
}
analyze_subset_selection_object(subset_selection_object)</pre>
```







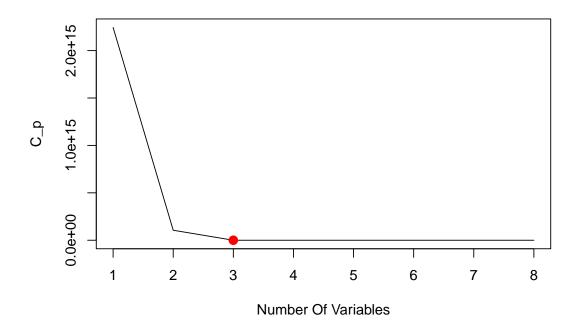
The best model obtained according to Mallow's  $C_p$ , the Schwartz Bayesian Information Criterion, and adjusted  $\mathbb{R}^2$  is

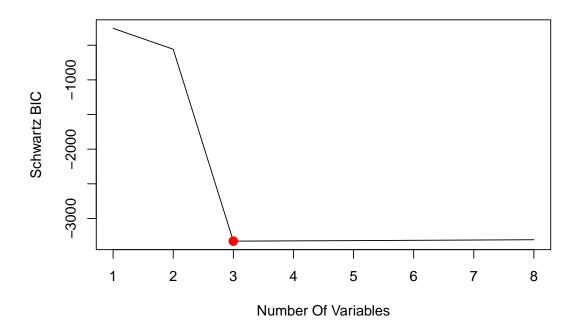
$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 = 1 + 2X + 3X^2 + 4X^3$$

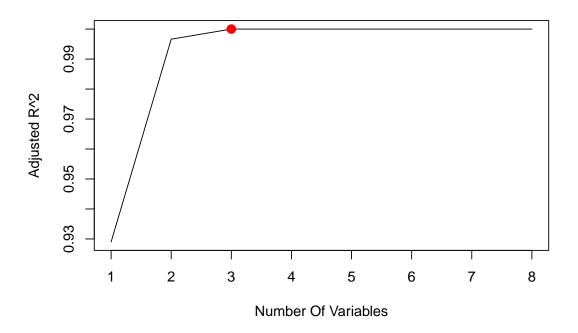
(d) Repeat (c), using forward stepwise selection and also using backwards stepwise selection. How does your answer compare to the results in (c)?

The models chosen by forward and backward selection involve the true predictive terms and their coefficients.

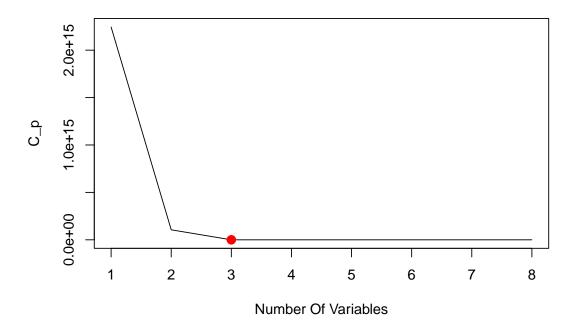
```
subset_selection_object <- regsubsets(
    x = formula,
    data = data_frame,
    method = "forward"
)
analyze_subset_selection_object(subset_selection_object)</pre>
```

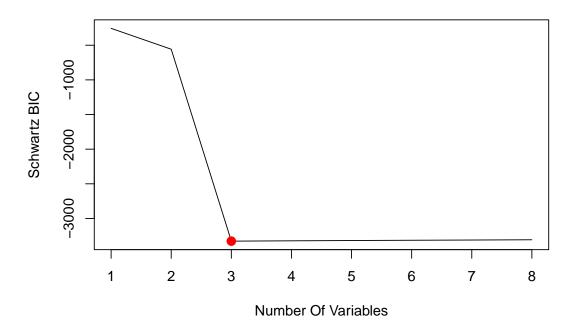


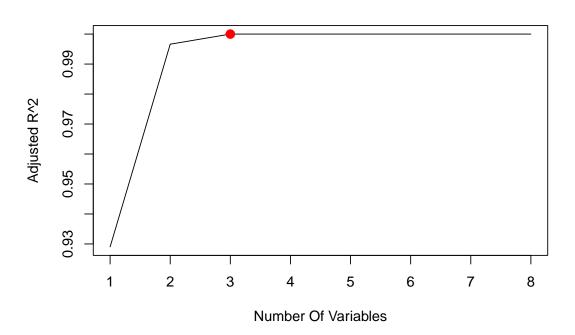




```
# $coefficients_by_Schwartz_BIC
# (Intercept)
                         Х
                                I(X^2)
                                            I(X^3)
                         2
            1
#
# $coefficients_by_adjusted_R2
# (Intercept)
                                I(X^2)
                                            I(X^3)
subset_selection_object <- regsubsets(</pre>
    x = formula,
    data = data_frame,
    method = "backward"
)
analyze_subset_selection_object(subset_selection_object)
```







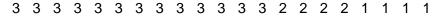
The best model obtained according to Mallow's  $C_p$ , the Schwartz Bayesian Information Criterion, and adjusted  $\mathbb{R}^2$  is

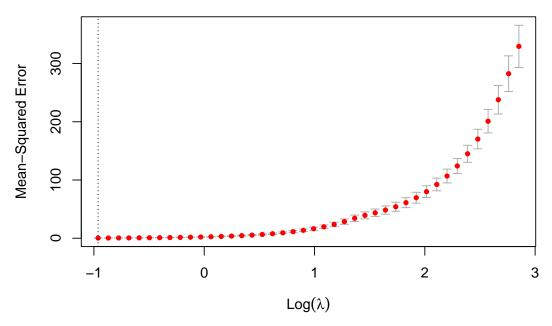
$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 = 1 + 2X + 3X^2 + 4X^3$$

These results are identical to those in part (c).

(e) Now fit a lasso model to the simulated data, again using  $X, X^2 \dots, X^{10}$  as predictors. Use cross-validation to select the optimal value of  $\lambda$ . Create plots of the cross-validation error as a function of  $\lambda$ . Report the resulting coefficient estimates, and discuss the results obtained.

```
full_model_matrix <- model.matrix(object = formula, data = data_frame)[, -1]
the_cv.glmnet <- glmnet::cv.glmnet(x = full_model_matrix, y = Y, alpha = 1)
plot(the_cv.glmnet)</pre>
```





```
optimal_value_of_lambda <- the_cv.glmnet$lambda.min
optimal_value_of_lambda</pre>
```

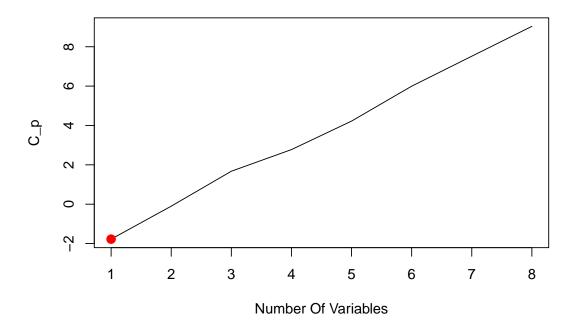
## # [1] 0.3822143

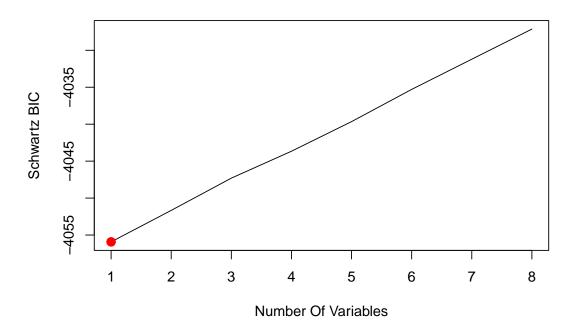
```
polynomial_lasso_regression_model <- glmnet::glmnet(full_model_matrix, y = Y, alpha = 1)
predict(object = polynomial_lasso_regression_model, s = optimal_value_of_lambda, type = "coeff")</pre>
```

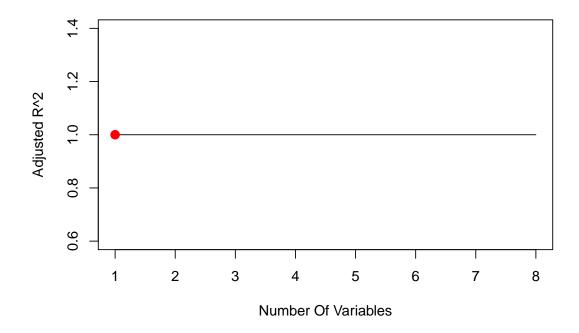
```
# 11 x 1 sparse Matrix of class "dgCMatrix"
                     s1
# (Intercept) 1.364119
# X
              1.990943
# I(X^2)
              2.730444
              3.899032
# I(X^3)
\# I(X^4)
\# I(X^5)
# I(X^6)
# I(X^7)
# I(X^8)
# I(X^9)
# I(X^10)
```

The models chosen by polynomial lasso regression involve the true predictive terms and rough approximations of their coefficients.  $\beta_0 = 1.364$ ,  $\beta_1 = 1.991$ ,  $\beta_2 = 2.730$ , and  $\beta_3 = 3.899$ .

(f) Now generate a response vector Y according to the model  $Y = \beta_0 + \beta_7 X^7 + \epsilon$ , and perform best subset selection and the lasso. Discuss the results obtained.





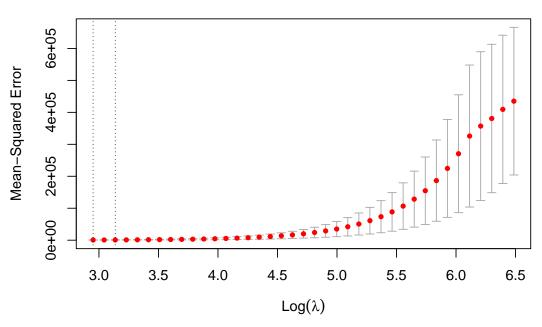


The best model obtained according to Mallow's  $C_p$ , the Schwartz Bayesian Information Criterion, and adjusted  $\mathbb{R}^2$  is

$$Y = \beta_0 + \beta_7 X^7 = 1 + 8X^7$$

full\_model\_matrix <- model.matrix(object = formula, data = data\_frame)[, -1]
the\_cv.glmnet <- glmnet::cv.glmnet(x = full\_model\_matrix, y = Y, alpha = 1)
plot(the\_cv.glmnet)</pre>





optimal\_value\_of\_lambda <- the\_cv.glmnet\$lambda.min

optimal\_value\_of\_lambda

7.7667958

# I(X^4) # I(X^5) # I(X^6)

# I(X^7) # I(X^8) # I(X^9) # I(X^10)

The models chosen by polynomial lasso regression involve the true predictive terms and rough approximations of their coefficients.  $\beta_0 = 1.364$  and  $\beta_7 = 7.767$ .

# 9. In this exercise, we will predict the number of applications received using the other variables in the College data set.

(a) Split the data set into a training set and a test set.

```
colleges <- ISLR2::College</pre>
head(colleges, n = 3)
                               Private Apps Accept Enroll Top10perc Top25perc
# Abilene Christian University
                                   Yes 1660
                                             1232
                                                      721
                                                                 23
# Adelphi University
                                   Yes 2186
                                             1924
                                                      512
                                                                 16
                                                                           29
                                   Yes 1428
                                             1097
                                                      336
                                                                 22
                                                                           50
# Adrian College
                               F.Undergrad P.Undergrad Outstate Room.Board Books
# Abilene Christian University
                                      2885
                                                  537
                                                          7440
                                                                     3300
# Adelphi University
                                      2683
                                                 1227
                                                          12280
                                                                      6450
                                                                            750
# Adrian College
                                      1036
                                                   99
                                                          11250
                                                                     3750 400
                              Personal PhD Terminal S.F.Ratio perc.alumni Expend
# Abilene Christian University
                                  2200 70 78
                                                        18.1 12 7041
# Adelphi University
                                  1500 29
                                                30
                                                         12.2
                                                                       16 10527
# Adrian College
                                   1165 53
                                                 66
                                                         12.9
                                                                       30 8735
                               Grad.Rate
# Abilene Christian University
                                     60
# Adelphi University
                                      56
# Adrian College
                                      54
proportion_of_training_data <- 0.9</pre>
library(TomLeversRPackage)
split_data <- split_data_set_into_training_and_testing_data(</pre>
    data_frame = colleges,
    proportion_of_training_data = proportion_of_training_data
vector_of_indices_of_training_data <- split_data$vector_of_indices_of_training_data
vector_of_indices_of_training_data[1:3]
# [1] 464 37 678
vector_of_indices_of_testing_data <- split_data$vector_of_indices_of_testing_data
vector_of_indices_of_testing_data[1:3]
# [1] 728 491 550
training_data <- split_data$training_data</pre>
head(training_data, n = 3)
                                    Private Apps Accept Enroll Top10perc
# Quincy University
                                       Yes 1025
                                                            297
                                                     707
                                                                       22
                                       Yes 1910
# Bard College
                                                    838
                                                            285
                                                                       50
# University of Southern California
                                       Yes 12229
                                                   8498
                                                          2477
                                                                       45
                                   Top25perc F.Undergrad P.Undergrad Outstate
# Quincy University
                                                    1070
                                                                72 10100
                                          66
# Bard College
                                           85
                                                     1004
                                                                  15
                                                                        19264
```

```
# University of Southern California
                                                     13259
                                                                   1429
                                                                           17230
#
                                     Room.Board Books Personal PhD Terminal
# Quincy University
                                           4140
                                                  450
                                                           1080 69
                                                                          71
# Bard College
                                           6206
                                                  750
                                                            750 98
                                                                          98
# University of Southern California
                                           6482
                                                  600
                                                          2210 90
                                                                          94
                                     S.F.Ratio perc.alumni Expend Grad.Rate
# Quincy University
                                          16.3
                                                        32
                                                              6880
# Bard College
                                          10.4
                                                        30
                                                            13894
                                                                          79
# University of Southern California
                                          11.4
                                                        10 17007
                                                                          68
```

```
testing_data <- split_data$testing_data
head(testing_data, n = 3)</pre>
```

```
Private Apps Accept Enroll Top10perc Top25perc
# Washington State University
                                         No 6540
                                                    5839
                                                           2440
                                                                       31
                                                                                 70
# Saint Francis College IN
                                        Yes 213
                                                    166
                                                             85
                                                                       13
                                                                                 36
# St. Mary's College of California
                                        Yes 2643
                                                   1611
                                                            465
                                                                       36
                                                                                 80
                                    F. Undergrad P. Undergrad Outstate Room. Board
# Washington State University
                                          14445
                                                       1344
                                                                 8200
# Saint Francis College IN
                                                                 8670
                                                                            3820
                                            513
                                                        247
# St. Mary's College of California
                                           2615
                                                        248
                                                                13332
                                                                            6354
                                    Books Personal PhD Terminal S.F.Ratio
# Washington State University
                                      800
                                              2719 84
                                                              87
# Saint Francis College IN
                                      450
                                              1000
                                                    43
                                                              78
                                                                      12.5
# St. Mary's College of California
                                      630
                                              1584 88
                                                                      16.1
                                    perc.alumni Expend Grad.Rate
# Washington State University
                                             30 10912
                                                               56
# Saint Francis College IN
                                                  7440
                                                               48
# St. Mary's College of California
                                                  9619
                                                               78
                                             17
```

(b) Fit a linear model using least squares on the training set, and report the test error obtained.

```
formula = Apps ~ .
linear_model <- lm(formula, data = training_data)
calculate_mean_squared_error(linear_model)</pre>
```

#### # [1] 1043968

```
y_hat_linear <- predict(
    object = linear_model,
    testing_data
)

testing_vector_of_numbers_of_applications <-
    colleges$Apps[vector_of_indices_of_testing_data]
y <- testing_vector_of_numbers_of_applications
y_bar <- mean(testing_vector_of_numbers_of_applications)
R_squared <- 1 - mean((y_hat_linear - y)^2) / mean((y_bar - y)^2)
R_squared</pre>
```

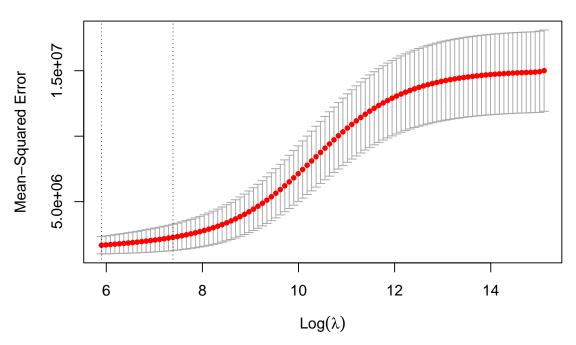
#### # [1] 0.8744088

The resulting mean squared error of prediction  $MSEP_{linear} = 1,043,968$ .

(c) Fit a ridge regression model on the training set, with  $\lambda$  chosen by cross-validation. Report the test error obtained.

```
full_model_matrix <- model.matrix(object = formula, data = colleges)[, -1]
the_cv.glmnet <- glmnet::cv.glmnet(
    x = full_model_matrix,
    y = colleges$Apps,
    alpha = 0
)
plot(the_cv.glmnet)</pre>
```

#### 



```
optimal_value_of_lambda <- the_cv.glmnet$lambda.min
optimal_value_of_lambda</pre>
```

#### # [1] 364.8993

```
training_data_frame <- colleges[vector_of_indices_of_training_data, ]
training_model_matrix <- model.matrix(
    object = formula,
    data = training_data_frame
)[, -1]
training_vector_of_numbers_of_applications <-
    colleges$Apps[vector_of_indices_of_training_data]
polynomial_ridge_regression_model <- glmnet::glmnet(
    x = training_model_matrix,
    y = training_vector_of_numbers_of_applications,</pre>
```

```
alpha = 0
)
testing_data_frame <- colleges[vector_of_indices_of_testing_data, ]</pre>
testing_model_matrix <- model.matrix(</pre>
    object = formula,
    data = testing_data_frame
)[, -1]
vector_of_predicted_numbers_of_applications <- predict(</pre>
    object = polynomial_ridge_regression_model,
    s = optimal_value_of_lambda,
    newx = testing_model_matrix
)[, 1]
vector_of_residuals <-</pre>
    vector_of_predicted_numbers_of_applications -
    testing_vector_of_numbers_of_applications
vector_of_squared_residuals <- vector_of_residuals^2</pre>
mean_squared_error <- mean(vector_of_squared_residuals)</pre>
mean_squared_error
```

## # [1] 1071002

```
y_hat_ridge <- vector_of_predicted_numbers_of_applications
R_squared <- 1 - mean((y_hat_ridge - y)^2) / mean((y_bar - y)^2)
R_squared</pre>
```

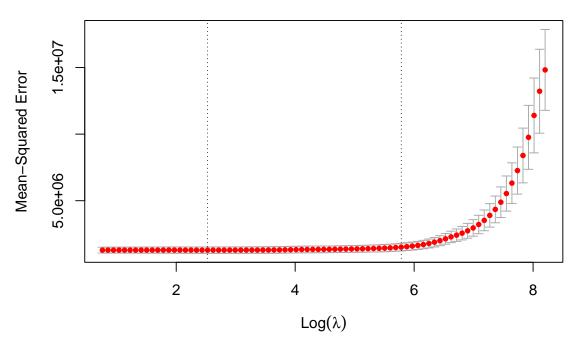
#### # [1] 0.8908082

The resulting mean squared error of prediction  $MSEP_{ridge} = 1,071,002$ .  $MSEP_{linear} < MSEP_{ridge}$ .

(d) Fit a lasso model on the training set, with  $\lambda$  chosen by cross-validation. Report the test error obtained, along with the number of non-zero coefficient estimates.

```
full_model_matrix <- model.matrix(object = formula, data = colleges)[, -1]
the_cv.glmnet <- glmnet::cv.glmnet(
    x = full_model_matrix,
    y = colleges$Apps,
    alpha = 1
)
plot(the_cv.glmnet)</pre>
```

## 17 17 17 15 15 10 9 5 4 3 3 3 2 2 1 1 1 1



```
optimal_value_of_lambda <- the_cv.glmnet$lambda.min
optimal_value_of_lambda</pre>
```

### # [1] 12.51776

```
training_model_matrix <- model.matrix(</pre>
    object = formula,
    data = training_data_frame
)[, -1]
training_vector_of_numbers_of_applications <-</pre>
    colleges$Apps[vector_of_indices_of_training_data]
testing_vector_of_numbers_of_applications <-</pre>
    colleges$Apps[vector_of_indices_of_testing_data]
polynomial_lasso_regression_model <- glmnet::glmnet(</pre>
    x = training_model_matrix,
    y = training_vector_of_numbers_of_applications,
    alpha = 1
testing_model_matrix <- model.matrix(</pre>
    object = formula,
    data = testing_data_frame
)[, -1]
vector_of_predicted_numbers_of_applications <- predict(</pre>
    object = polynomial_lasso_regression_model,
    s = optimal_value_of_lambda,
    newx = testing_model_matrix
```

```
)[, 1]
vector_of_residuals <-</pre>
    vector_of_predicted_numbers_of_applications -
    testing_vector_of_numbers_of_applications
vector_of_squared_residuals <- vector_of_residuals^2</pre>
mean_squared_error <- mean(vector_of_squared_residuals)</pre>
mean_squared_error
# [1] 1168351
predict(
    object = polynomial_lasso_regression_model,
    s = optimal_value_of_lambda,
    type = "coefficients"
)
# 18 x 1 sparse Matrix of class "dgCMatrix"
# (Intercept) -4.772317e+02
# PrivateYes -4.945991e+02
# Accept
               1.550834e+00
# Enroll
              -4.885202e-01
# Top10perc
               3.994779e+01
# Top25perc -5.578160e+00
# F.Undergrad 1.402583e-03
# P.Undergrad 4.404712e-02
# Outstate
             -7.179337e-02
# Room.Board 1.435632e-01
               6.641890e-02
# Books
# Personal
              9.897576e-03
# PhD
              -6.550167e+00
# Terminal -3.749746e+00
# S.F.Ratio
               4.409518e+00
# perc.alumni -1.416008e-01
# Expend
               6.819184e-02
# Grad.Rate
                6.068215e+00
y_hat_lasso <- vector_of_predicted_numbers_of_applications</pre>
R_{\text{squared}} \leftarrow 1 - \text{mean}((y_{\text{hat}}_{\text{lasso}} - y)^2) / \text{mean}((y_{\text{bar}} - y)^2)
R_squared
```

#### # [1] 0.8808833

The number of non-zero coefficients M=17, which is equal to the number of non-zero coefficients. The resulting mean squared error of prediction  $MSEP_{lasso}=1,168,351$ .  $MSEP_{linear} < MSEP_{ridge} < MSEP_{lasso}$ .

(e) Fit a PCR model on the training set, with M chosen by cross-validation. Report the test error obtained, along with the value of M selected by cross-validation.

```
library(pls)
```

```
# Warning: package 'pls' was built under R version 4.3.1

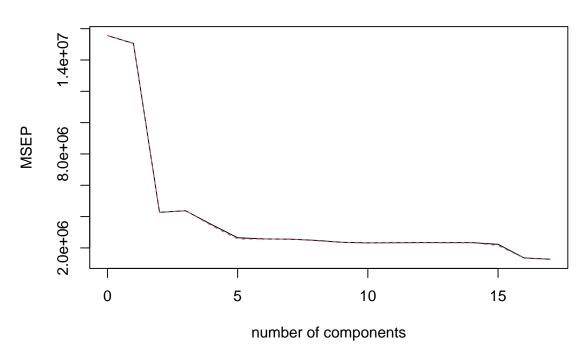
# 
# Attaching package: 'pls'

# The following object is masked from 'package:stats':

# 
loadings

the_mvr <- pcr(formula, data = training_data_frame, scale = TRUE, validation = "CV")
validationplot(the_mvr, val.type = "MSEP")</pre>
```

# **Apps**



```
vector_of_predicted_numbers_of_applications <- predict(
   object = the_mvr,
   testing_data_frame,
   ncomp = 17
)
vector_of_residuals <-
   vector_of_predicted_numbers_of_applications -
   testing_vector_of_numbers_of_applications
vector_of_squared_residuals <- vector_of_residuals^2
mean_squared_error <- mean(vector_of_squared_residuals)
mean_squared_error</pre>
```

# [1] 1231856

```
y_hat_PCR <- vector_of_predicted_numbers_of_applications
R_squared <- 1 - mean((y_hat_PCR - y)^2) / mean((y_bar - y)^2)
R_squared</pre>
```

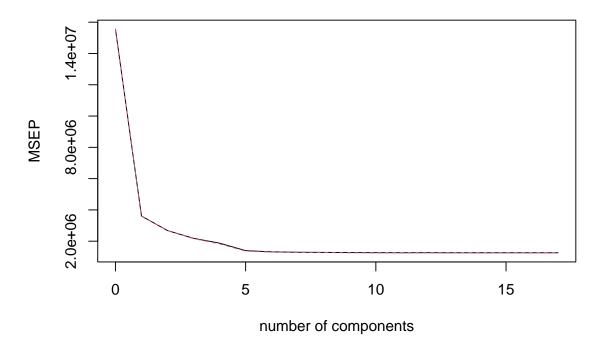
#### # [1] 0.8744088

The resulting mean squared error of prediction  $MSEP_{PCR} = 1,231,856.$   $MSEP_{linear} < MSEP_{ridge} < MSEP_{lasso} < MSEP_{PCR}.$ 

(f) Fit a PLS model on the training set, with M chosen by cross-validation. Report the test error obtained, along with the value of M selected by cross-validation.

```
library(pls)
the_mvr <- plsr(formula, data = training_data_frame, scale = TRUE, validation = "CV")
validationplot(the_mvr, val.type = "MSEP")</pre>
```

# **Apps**



vector\_of\_predicted\_numbers\_of\_applications <- predict(
 object = the\_mvr,
 testing\_data\_frame,
 ncomp = 17
)
vector\_of\_residuals < vector\_of\_predicted\_numbers\_of\_applications testing\_vector\_of\_numbers\_of\_applications
vector\_of\_squared\_residuals <- vector\_of\_residuals^2
mean\_squared\_error <- mean(vector\_of\_squared\_residuals)
mean\_squared\_error</pre>

#### # [1] 1231856

```
y_hat_PLSR <- vector_of_predicted_numbers_of_applications
R_squared <- 1 - mean((y_hat_PLSR - y)^2) / mean((y_bar - y)^2)
R_squared</pre>
```

#### # [1] 0.8744088

The number of non-zero coefficients estimates is 17. The resulting mean squared error of prediction  $MSEP_{PLSR} = 1,231,856$ .  $MSEP_{linear} < MSEP_{ridge} < MSEP_{lasso} < MSEP_{PCR}; MSEP_{PCR} = MSEP_{PLSR}$ .

(g) Comment on the results obtained. How accurately can we predict the number of college applications received? Is there much difference among the test errors resulting from these five approaches?

As above,  $MSEP_{linear} < MSEP_{ridge} < MSEP_{lasso} < MSEP_{PCR}; MSEP_{PCR} = MSEP_{PLSR}$ . The mean squared error of prediction of the linear model  $MSEP_{linear} = 1,043,968$ . The mean squared error of prediction of the PLSR model  $MSEP_{PLSR} = 1,231,856$ . The rate of difference between these errors is -0.153. There is a strong effect for each model;  $R^2_{linear} = R^2_{PCR} = R^2_{PLSR}; R^2_{linear} < R^2_{lasso} < R^2_{ridge}$ .