

# Bruce Campbell ST-617 Homework 2

Tue Jul 12 09:44:26 2016

## Chapter 6

### Problem 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  $n = 100$ .

```
rm(list = ls())
set.seed(123)
X <- rnorm(100, mean = 0, sd = 1)

epsilon <- rnorm(100, mean = 0, sd = 1)
```

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.

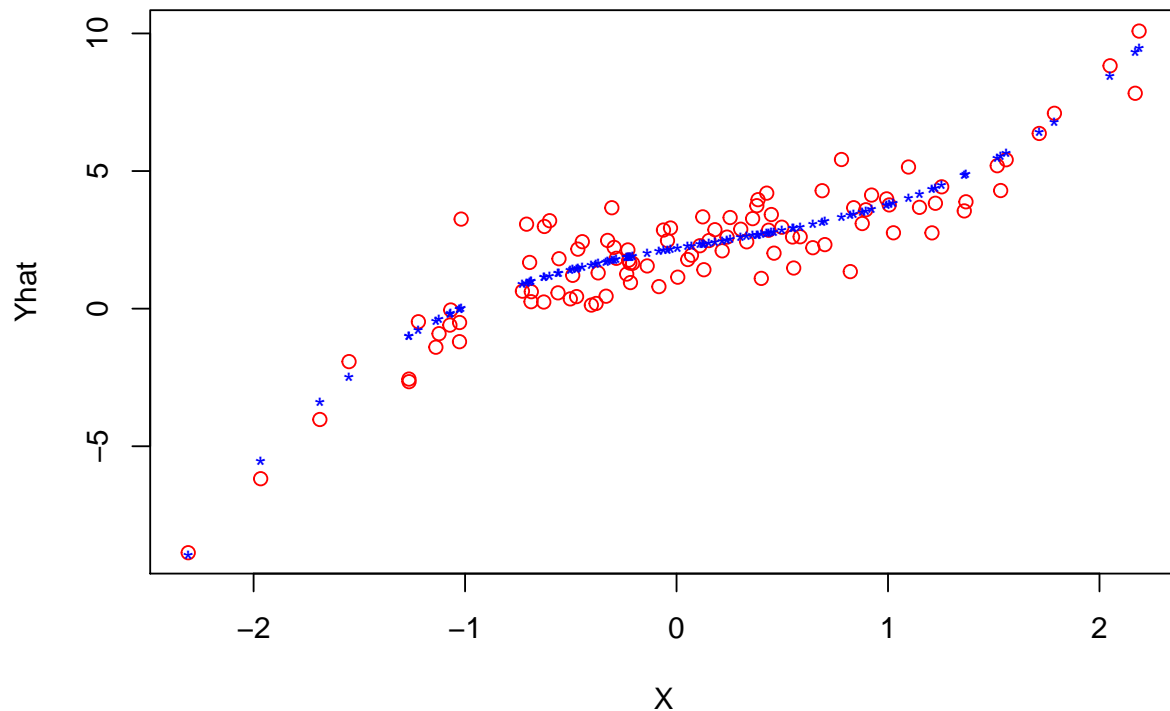
```
beta = rnorm(4, mean = 0, sd = 1)
Y <- matrix(NA, nrow = 100, ncol = 1)
Yhat <- matrix(NA, nrow = 100, ncol = 1)

for (i in 1:100) {
  Y[i] = beta[1] + beta[2] * X[i] + beta[3] * X[i]^2 + beta[4] * X[i]^3

  Yhat[i] = beta[1] + beta[2] * X[i] + beta[3] * X[i]^2 + beta[4] * X[i]^3 +
    epsilon[i]
}

plot(X, Yhat, col = "red")
points(X, Y, pch = "*", col = "blue")
title(main = sprintf("Y = %f + %f X + %f X^2+ %f X^3", beta[1], beta[2], +beta[3],
  beta[4]), cex = 4.6)
```

$$Y = 2.198810 + 1.312413 X + -0.265145 X^2 + 0.543194 X^3$$



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  $Y$ .

```
DF <- as.data.frame(X)
DF <- cbind(DF, Yhat)
names(DF) = c("X", "Y")
library(leaps)

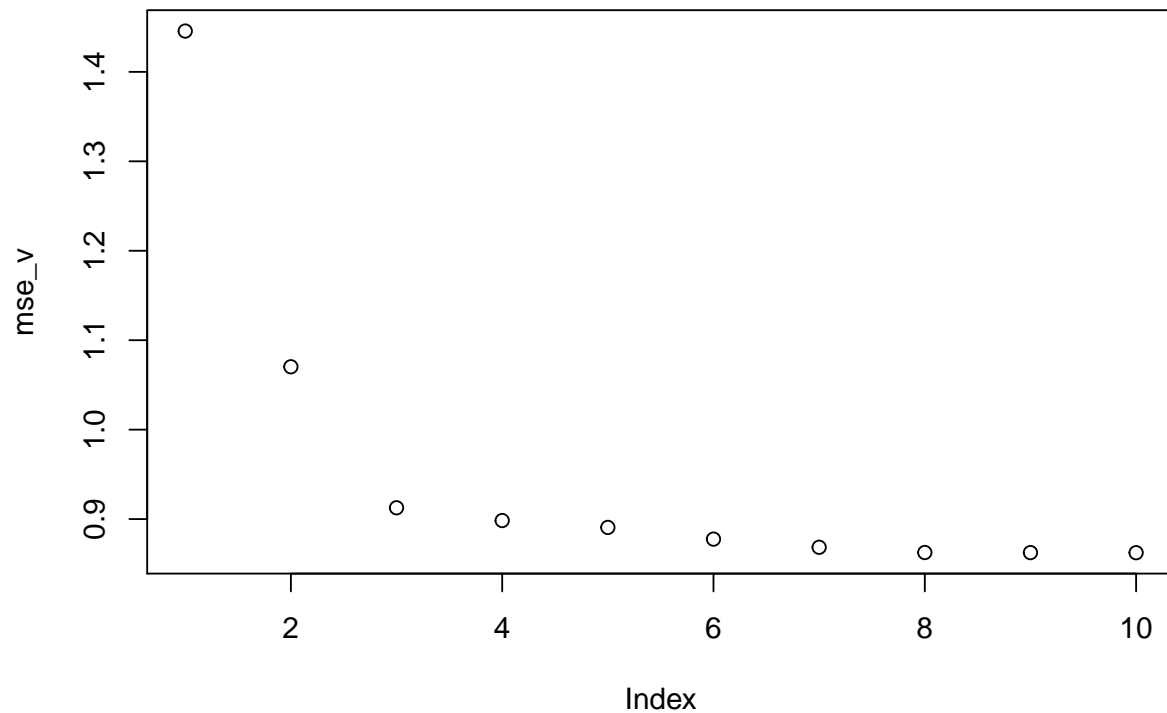
regfit.full <- regsubsets(Y ~ X + I(X^2) + I(X^3) + I(X^4) + I(X^5) + I(X^6) +
  I(X^7) + I(X^8) + I(X^9) + I(X^10), data = DF, nvmax = 10)

reg.summary <- summary(regfit.full)

mse_v <- reg.summary$rss/nrow(DF)

plot(mse_v)
title("MSE versus model size for best subset selection algorithm on training set.")
```

## MSE versus model size for best subset selection algorithm on training se



We see that there is a sharp drop in the training set  $MSE$  until 3 or 4 predictors are included and that there is a steady decrease as additional polynomial terms are included. This is attributed to over fitting to the training data.

```
summary(regfit.full)
```

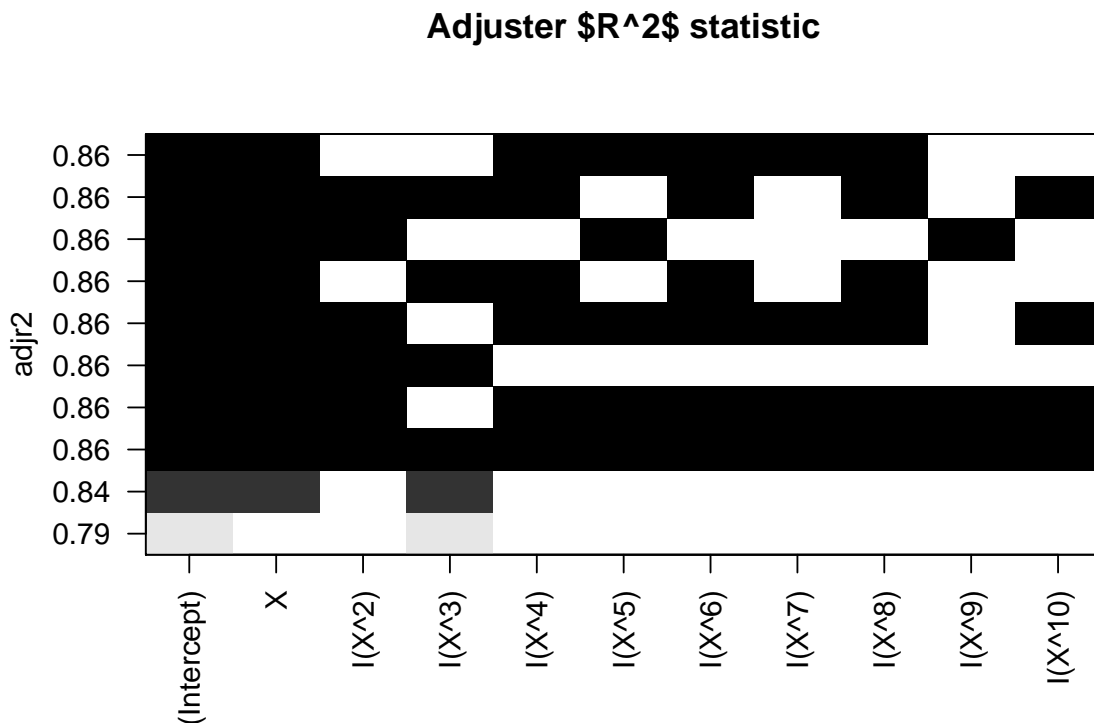
```
## Subset selection object
## Call: regsubsets.formula(Y ~ X + I(X^2) + I(X^3) + I(X^4) + I(X^5) +
##       I(X^6) + I(X^7) + I(X^8) + I(X^9) + I(X^10), data = DF, nvmax = 10)
## 10 Variables (and intercept)
##           Forced in Forced out
## X                FALSE      FALSE
## I(X^2)            FALSE      FALSE
## I(X^3)            FALSE      FALSE
## I(X^4)            FALSE      FALSE
## I(X^5)            FALSE      FALSE
## I(X^6)            FALSE      FALSE
## I(X^7)            FALSE      FALSE
## I(X^8)            FALSE      FALSE
## I(X^9)            FALSE      FALSE
## I(X^10)           FALSE      FALSE
## 1 subsets of each size up to 10
## Selection Algorithm: exhaustive
##           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)
## 1  ( 1 )  " " " "  "*"  " "  " "  " "  " "  " "
```

```

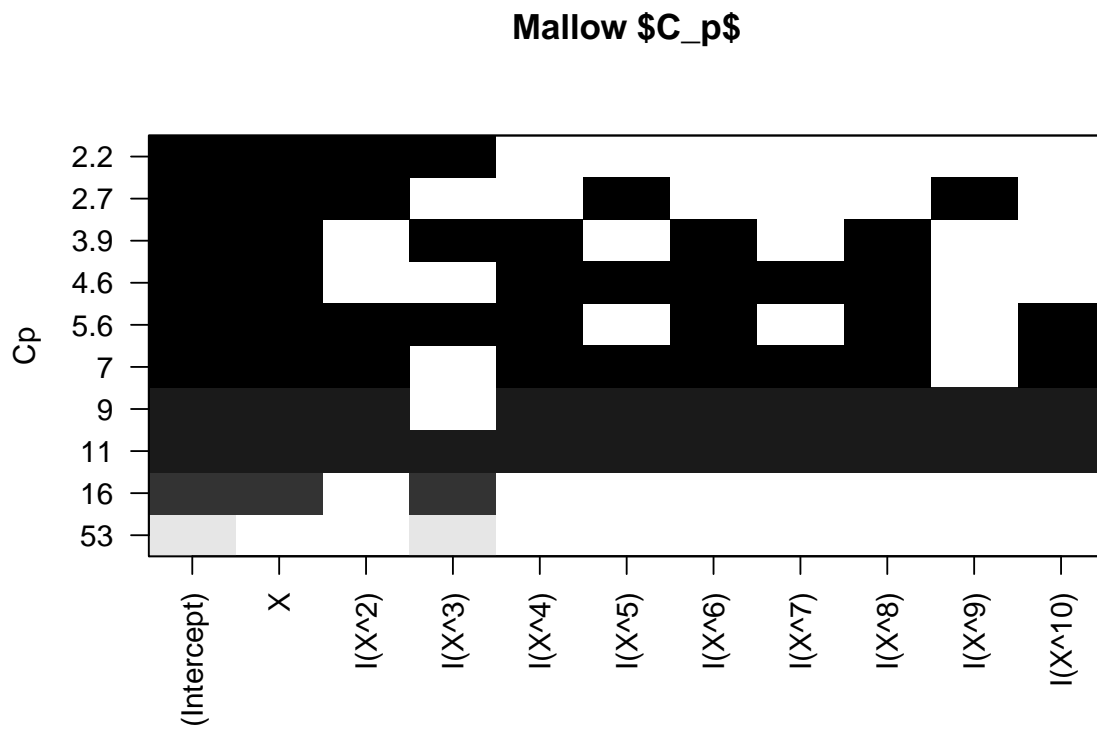
## 2 ( 1 ) "*" " " "*" " " " " " " " " " "
## 3 ( 1 ) "*" "*" "*" " " " " " " " " " "
## 4 ( 1 ) "*" "*" " " " " "*" " " " " "*"
## 5 ( 1 ) "*" " " "*" "*" " " "*" " " "*" " "
## 6 ( 1 ) "*" " " " " "*" "*" "*" "*" "*" " "
## 7 ( 1 ) "*" "*" "*" "*" " " "*" " " "*" " "
## 8 ( 1 ) "*" "*" " " "*" "*" "*" "*" "*" " "
## 9 ( 1 ) "*" "*" " " "*" "*" "*" "*" "*" "*"
## 10 ( 1 ) "*" "*" "*" "*" "*" "*" "*" "*" "*"
##      I(X^10)
## 1 ( 1 ) " "
## 2 ( 1 ) " "
## 3 ( 1 ) " "
## 4 ( 1 ) " "
## 5 ( 1 ) " "
## 6 ( 1 ) " "
## 7 ( 1 ) "*"
## 8 ( 1 ) "*"
## 9 ( 1 ) "*"
## 10 ( 1 ) "*"

```

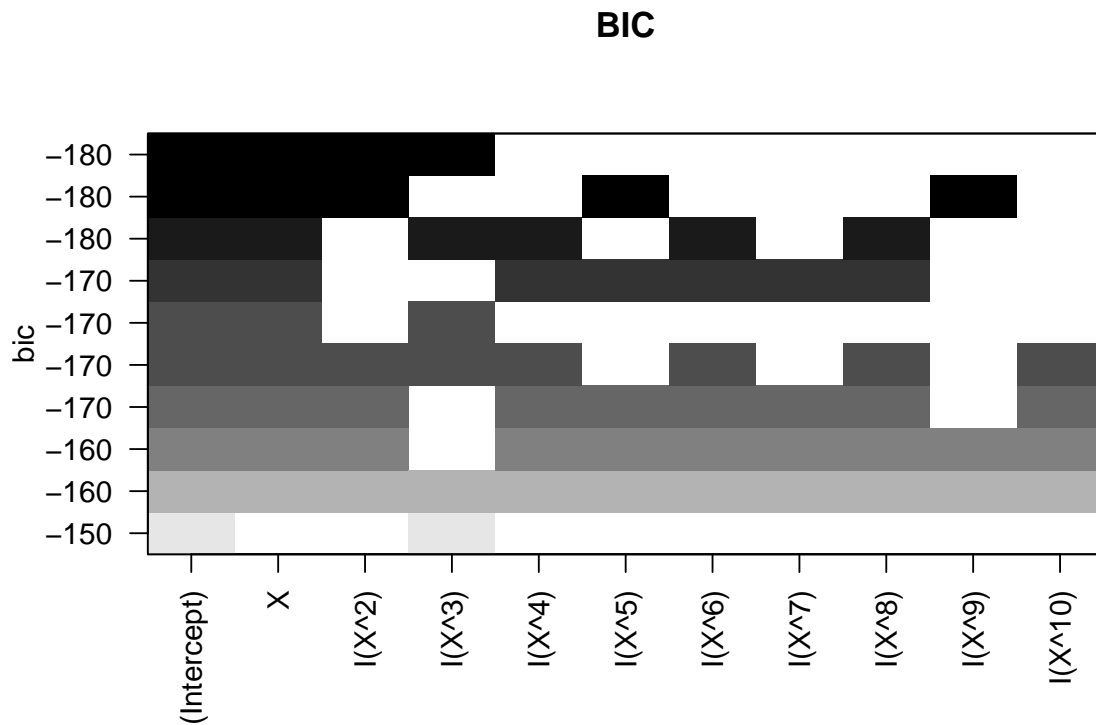
We notice the best subset algorithm has correctly included the proper terms in the third sets of predictors.



We need to remember that with  $R^2$  statistic the values closer to 1 are a better fit. Among those with a value of 0.86 we see that the model with *Intercept*,  $X$ ,  $X^2$ ,  $X^3$  is selected.



The  $C_p$  statistic indicates that the best model contains *Intercept*,  $X$ ,  $X^2$ ,  $X^3$



The *BIC* statistic indicates that the best model contains *Intercept*,  $X$ ,  $X^2$ ,  $X^3$

There was a problem with knitr where the cache was corrupted and the plots from old models were included. The section below is retained for that purpose.

```
beta_test <- matrix(NA, nrow = 4, ncol = 1)
beta_test[1] = 1
beta_test[2] = 6
beta_test[3] = 0.6
beta_test[4] = 0.6

Y_test <- matrix(NA, nrow = 100, ncol = 1)
Yhat_test <- matrix(NA, nrow = 100, ncol = 1)

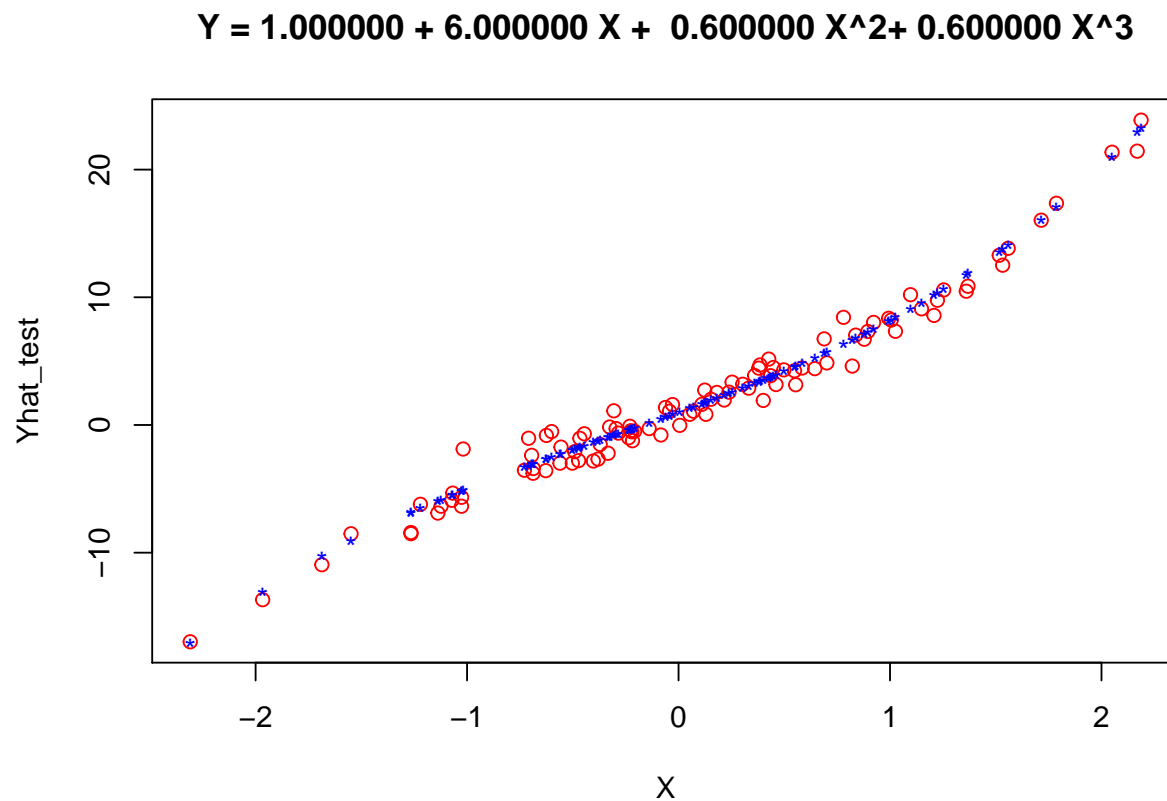
for (i in 1:100) {
  Y_test[i] = beta_test[1] + beta_test[2] * X[i] + beta_test[3] * X[i]^2 +
    beta_test[4] * X[i]^3

  Yhat_test[i] = beta_test[1] + beta_test[2] * X[i] + beta_test[3] * X[i]^2 +
    beta_test[4] * X[i]^3 + epsilon[i]
}

DF_test <- as.data.frame(X)
DF_test <- cbind(DF, Yhat_test)
names(DF) = c("X", "Y")

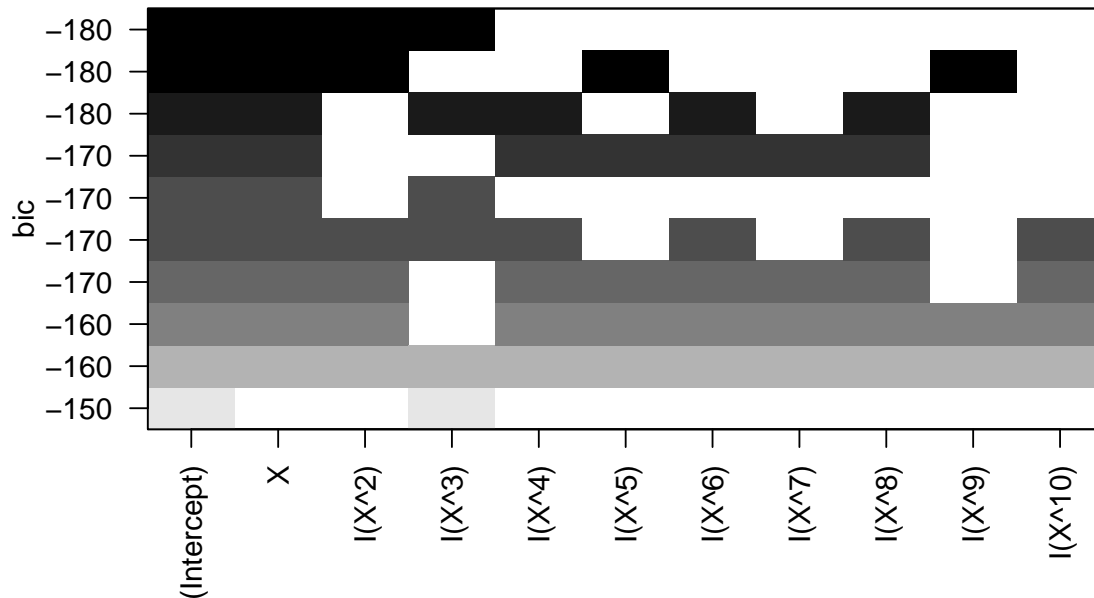
plot(X, Yhat_test, col = "red")
```

```
points(X, Y_test, pch = "*", col = "blue")
title(main = sprintf("Y = %f + %f X + %f X^2+ %f X^3", beta_test[1], beta_test[2],
+beta_test[3], beta_test[4]), cex = 4.6)
```



```
regfit.full <- regsubsets(Y ~ 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^10), data = DF_test, nvmax = 10)
plot(regfit.full, scale = "bic")
title("BIC - for model with strong linear component ")
```

## BIC – for model with strong linear component



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

### FORWARD SSS

```
regfit.full <- regsubsets(Y ~ 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^10), data = DF, nvmax = 10, method = "forward")

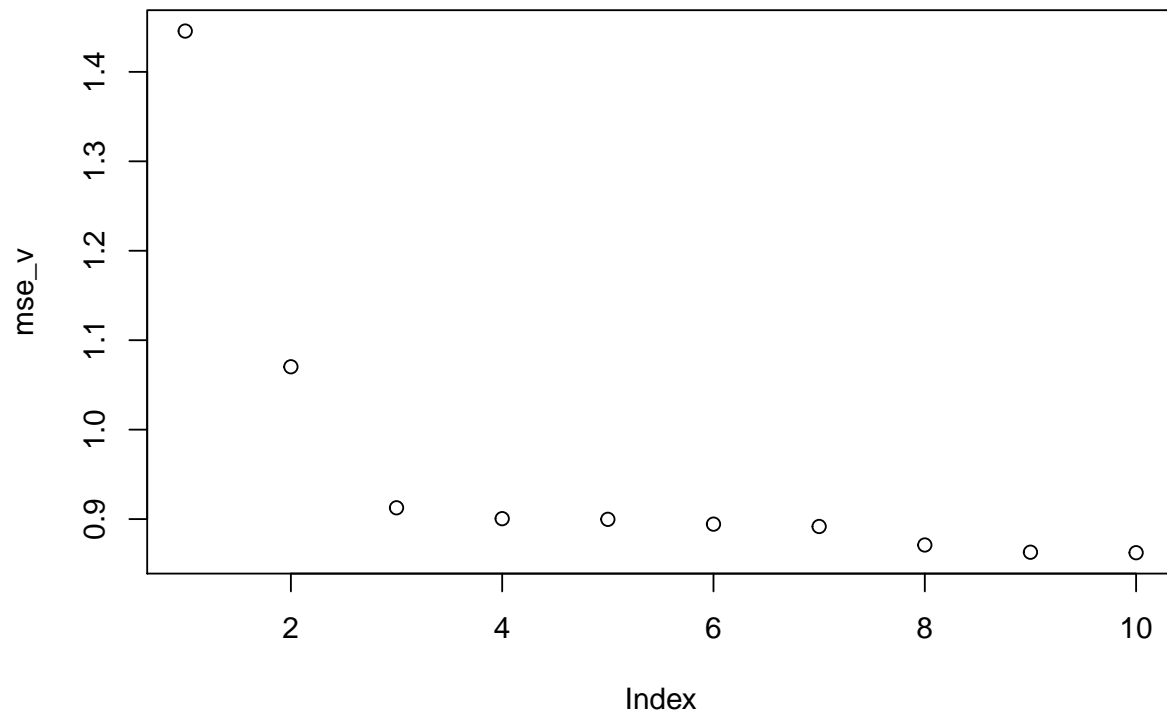
reg.summary <- summary(regfit.full)

mse_v <- reg.summary$rss/nrow(DF)

plot(mse_v)
title(c("MSE versus model size for forward subset selection algorithm on training set.",
  "Forward SSS"))
```

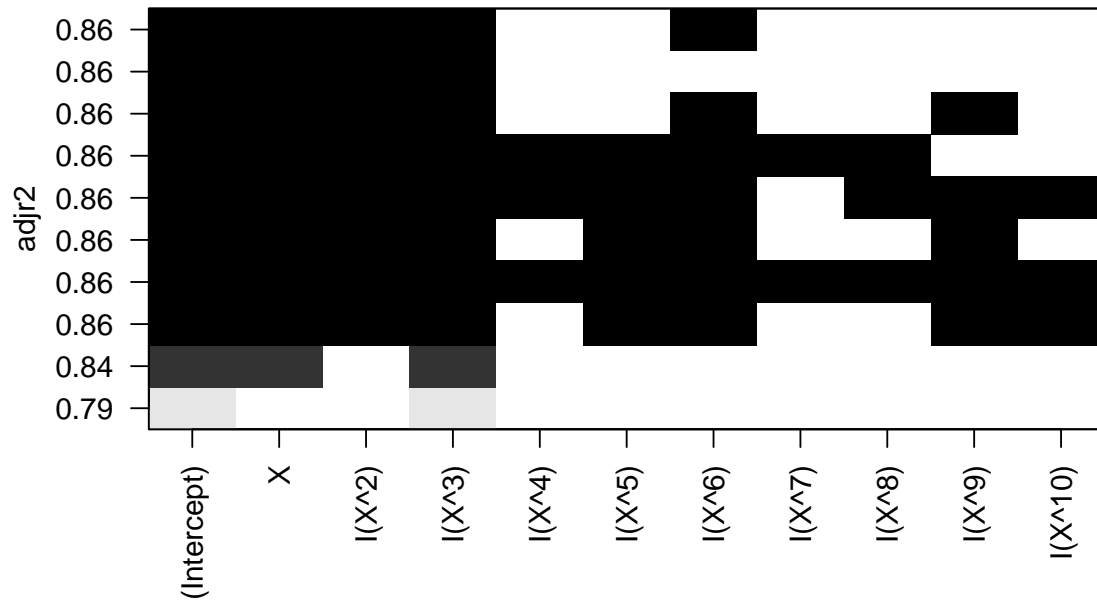


### MSE versus model size for forward subset selection algorithm on training : Forward SSS



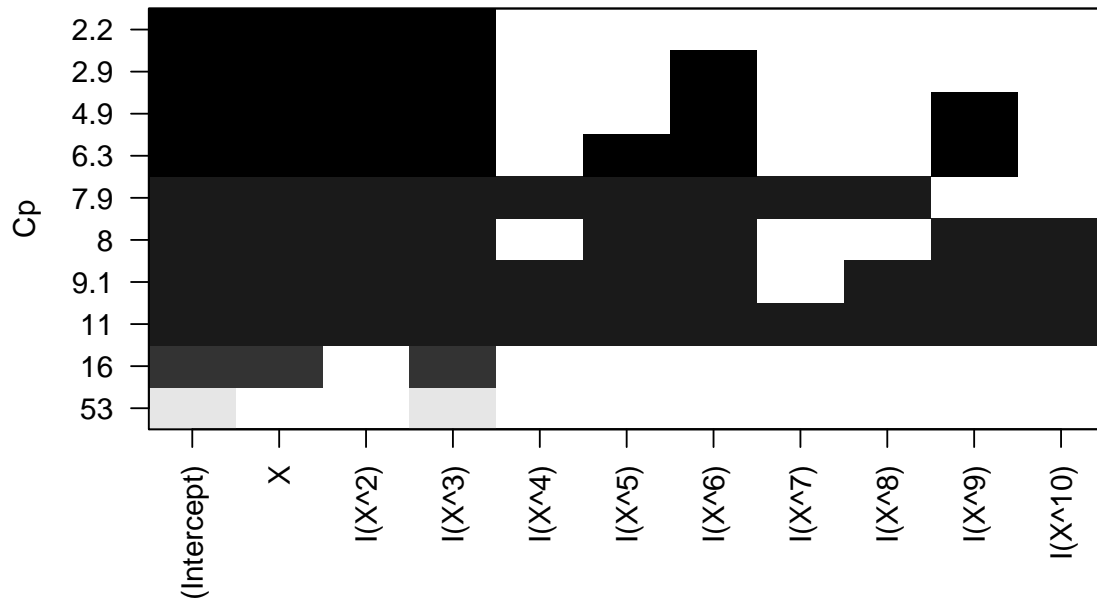
We see that there is a sharp drop in the training set  $MSE$  until 3 or 4 predictors are included and there is a steady decrease as additional polynomial terms are included. This is attributed to over fitting to the training data.

### Adjuster $R^2$ statistic Forward SSS



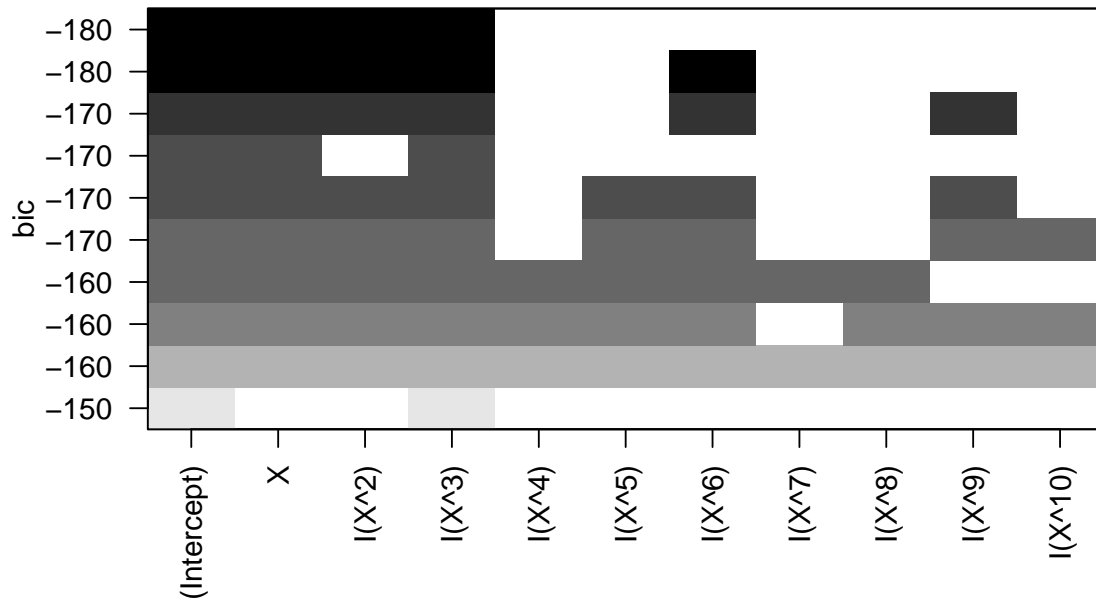
Among those with a value of 0.86 we see that the model with *Intercept*,  $X$ ,  $X^2$ ,  $X^3$  is selected.

### Mallow $C_p$ Forward SSS



The  $C_p$  statistic indicates that the best model contains *Intercept*,  $X$ ,  $X^2$ ,  $X^3$

## BIC Forward SSS



The *BIC* statistic indicates that the best model contains *Intercept*,  $X$ ,  $X^2$ ,  $X^3$

## BACKWARD SSS

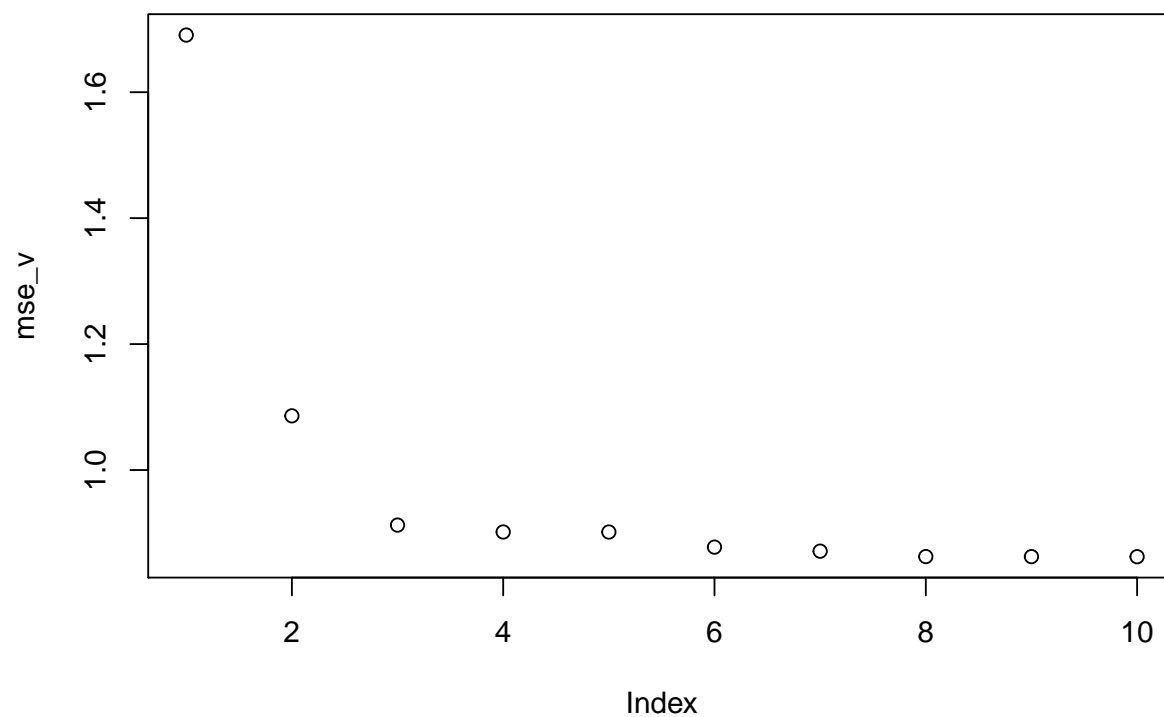
```
regfit.full <- regsubsets(Y ~ X + I(X^2) + I(X^3) + I(X^4) + I(X^5) + I(X^6) +
  I(X^7) + I(X^8) + I(X^9) + I(X^10), data = DF, nvmax = 10, method = "backward")

reg.summary <- summary(regfit.full)

mse_v <- reg.summary$rss/nrow(DF)

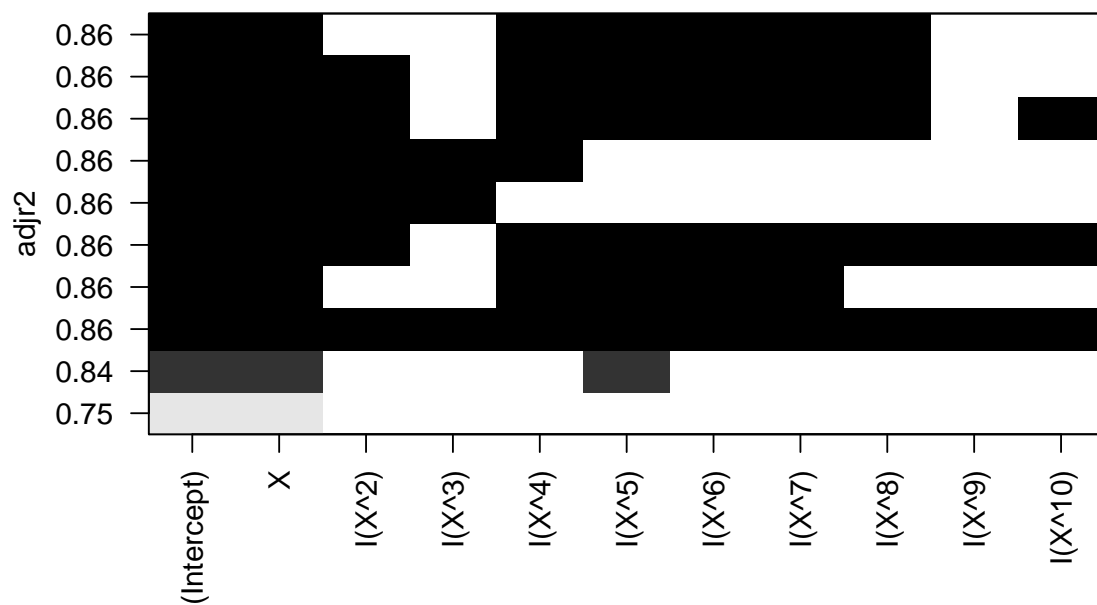
plot(mse_v)
title(c("MSE versus model size for backward subset selection algorithm on training set.",
  "Backward SSS"))
```

### MSE versus model size for backward subset selection algorithm on training Backward SSS



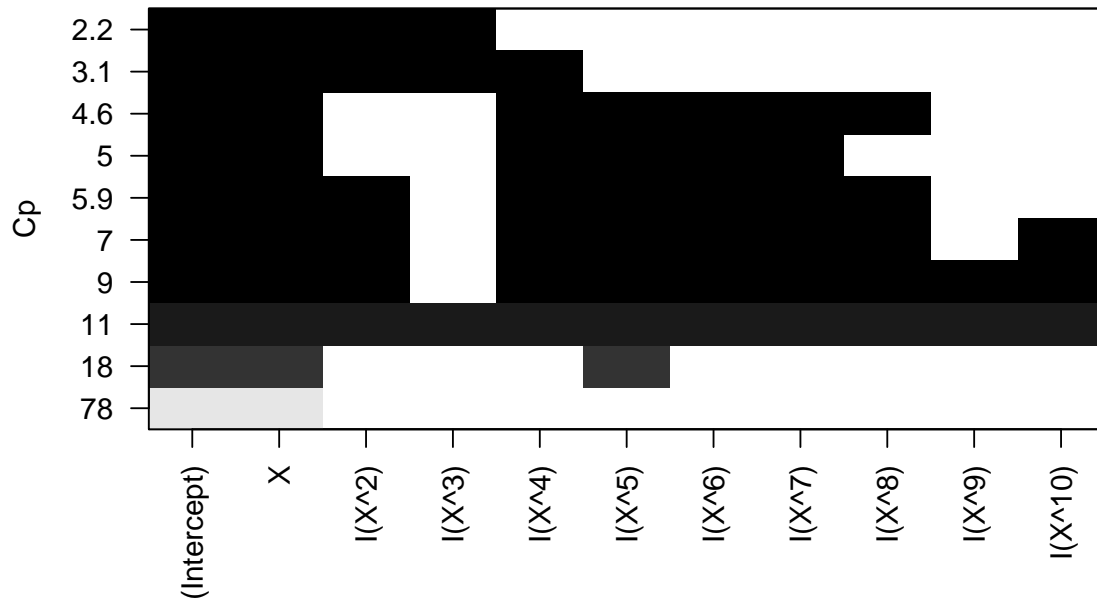
We see that there is a sharp drop in the training set  $MSE$  until 2 predictors are included and there is a steady decrease as additional polynomial terms are included. This is attributed to over fitting to the training data.

### Adjuster $R^2$ statistic Backward SSS

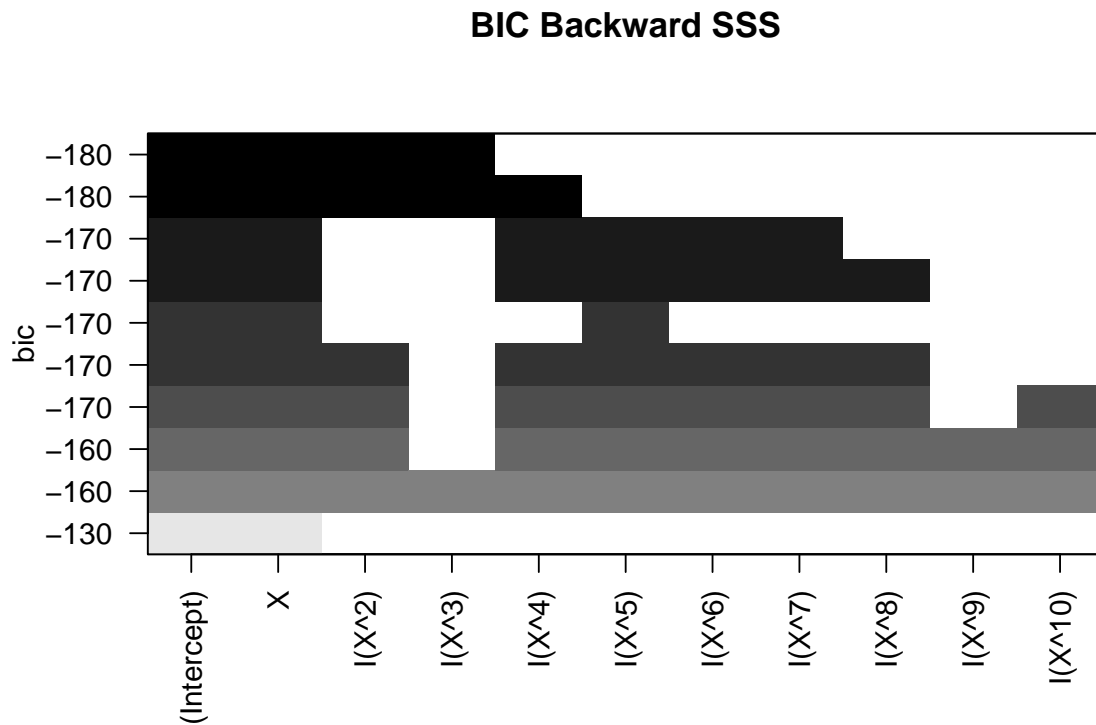


We need to remember that with  $R^2$  statistic the values closer to 1 are a better fit. Among those with a value of 0.86 we see the full model (*Intercept*),  $X$ ,  $X^2$ ,  $X^3$  has been selected.

### Mallow $C_p$ Backward SSS



The  $C_p$  statistic indicates that the best model contains  $(Intercept), X, X^2, X^3$



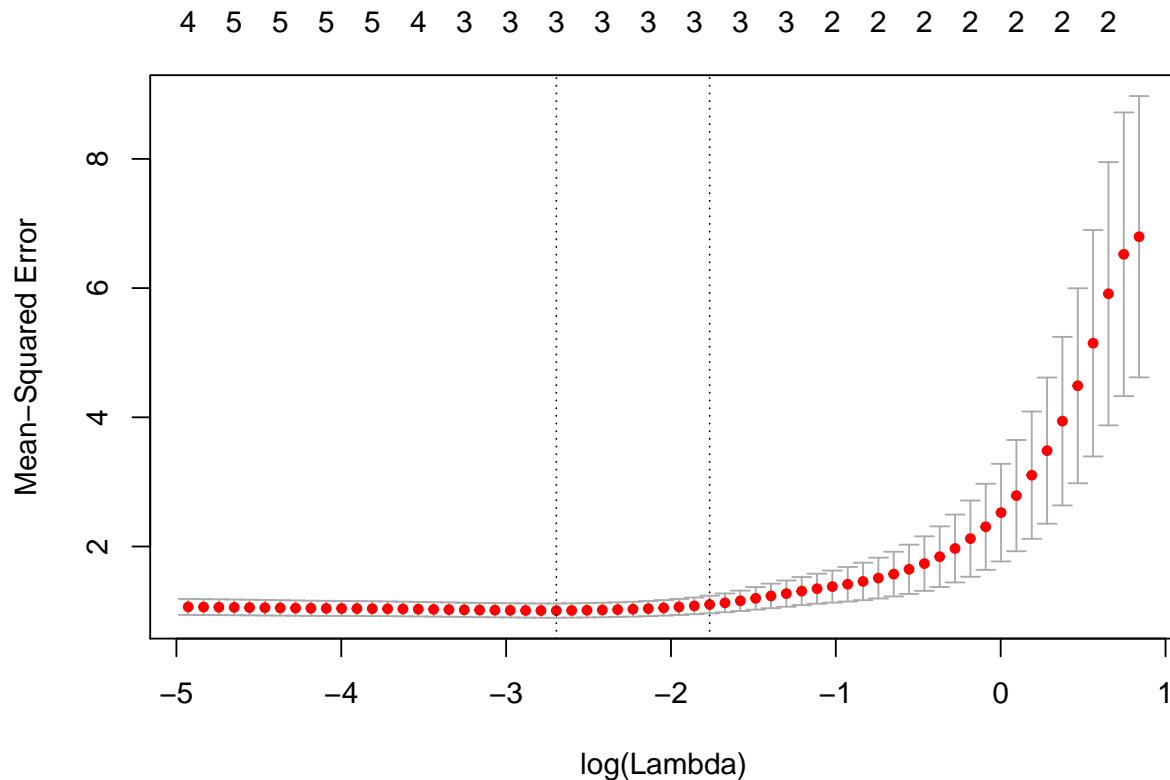
The *BIC* statistic indicates that the best model contains  $(Intercept), X, X^2, X^3$

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.

```
library(glmnet)
x_lasso = model.matrix(Y ~ 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^10), DF)[, -1]
y_lasso = DF$Y
cv.out = cv.glmnet(x_lasso, y_lasso, alpha = 1)
plot(cv.out)
```





```
bestlam = cv.out$lambda.min
bestlam
```

```
## [1] 0.06750938
```

```
best_lasso = glmnet(x_lasso, y_lasso, alpha = 1, lambda = bestlam)
predict(best_lasso, type = "coefficients", s = bestlam)[1:10, ]
```

```
## (Intercept)      X      I(X^2)      I(X^3)      I(X^4)      I(X^5)
##  2.1157969  1.1876459 -0.2813453  0.5440925  0.0000000  0.0000000
##      I(X^6)      I(X^7)      I(X^8)      I(X^9)
##  0.0000000  0.0000000  0.0000000  0.0000000
```

We see that the lasso for a value of lambda given by cross validation has driven all the extra model coefficients to 0 as expected.

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.

```

beta = rnorm(2, mean = 0, sd = 1)
Y <- matrix(NA, nrow = 100, ncol = 1)
Yhat <- matrix(NA, nrow = 100, ncol = 1)

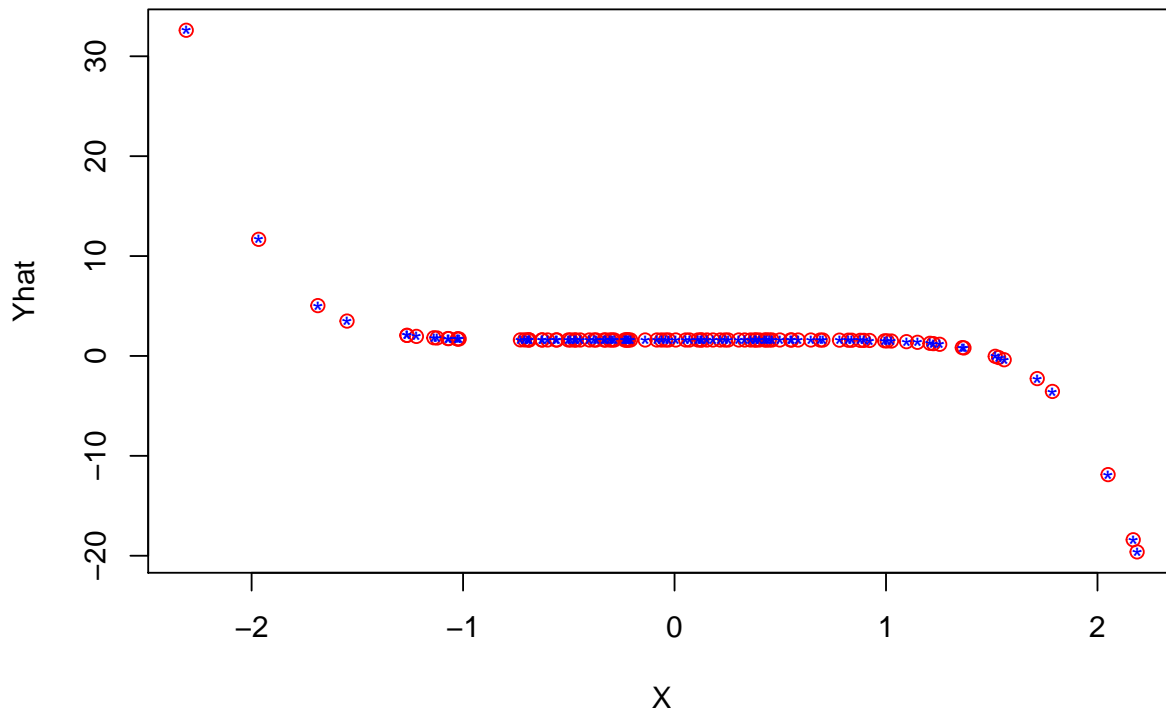
for (i in 1:100) {
  Y[i] = beta[1] + beta[2] * X[i]^7

  Yhat[i] = beta[1] + beta[2] * X[i]^7
}

plot(X, Yhat, col = "red")
points(X, Y, pch = "*", col = "blue")
title(main = sprintf("Y = %f + %f X^7", beta[1], beta[2]), cex = 4.6)

```

$$Y = 1.598509 + -0.088565 X^7$$



```

DF <- as.data.frame(X)
DF <- cbind(DF, Yhat)
names(DF) = c("X", "Y")
library(leaps)

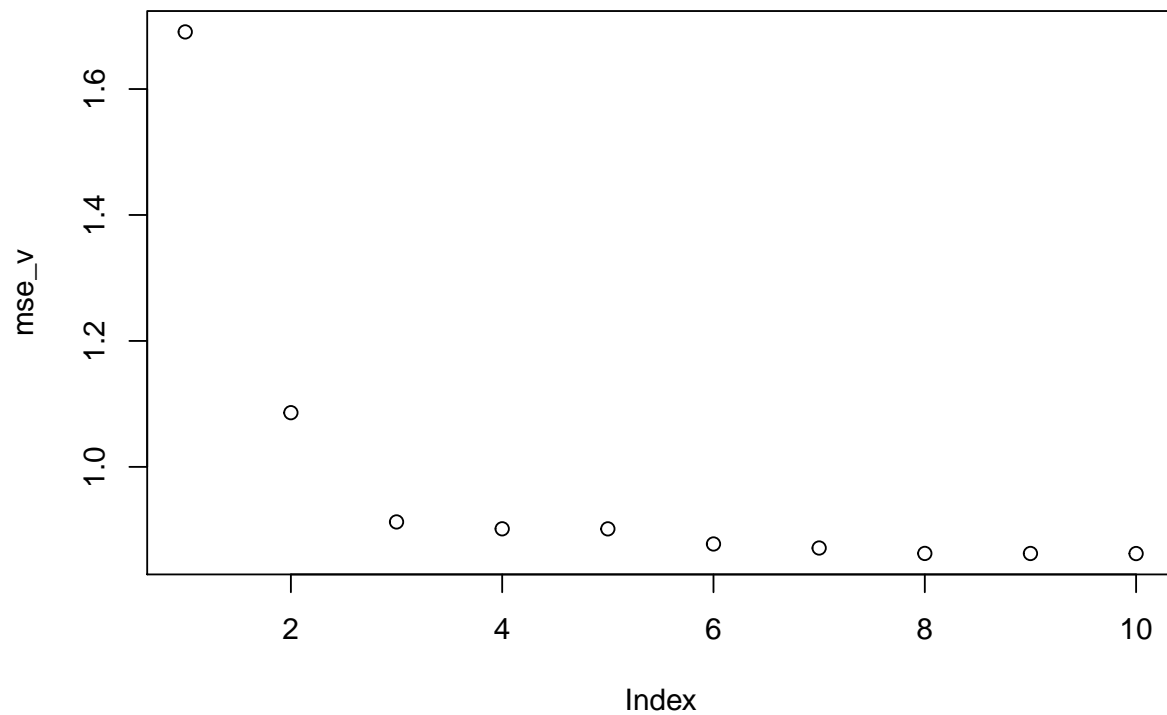
regfit.full <- regsubsets(Y ~ X + I(X^2) + I(X^3) + I(X^4) + I(X^5) + I(X^6) +
  I(X^7) + I(X^8) + I(X^9) + I(X^10), data = DF, nvmax = 10)

reg.summary <- summary(regfit.full)

```

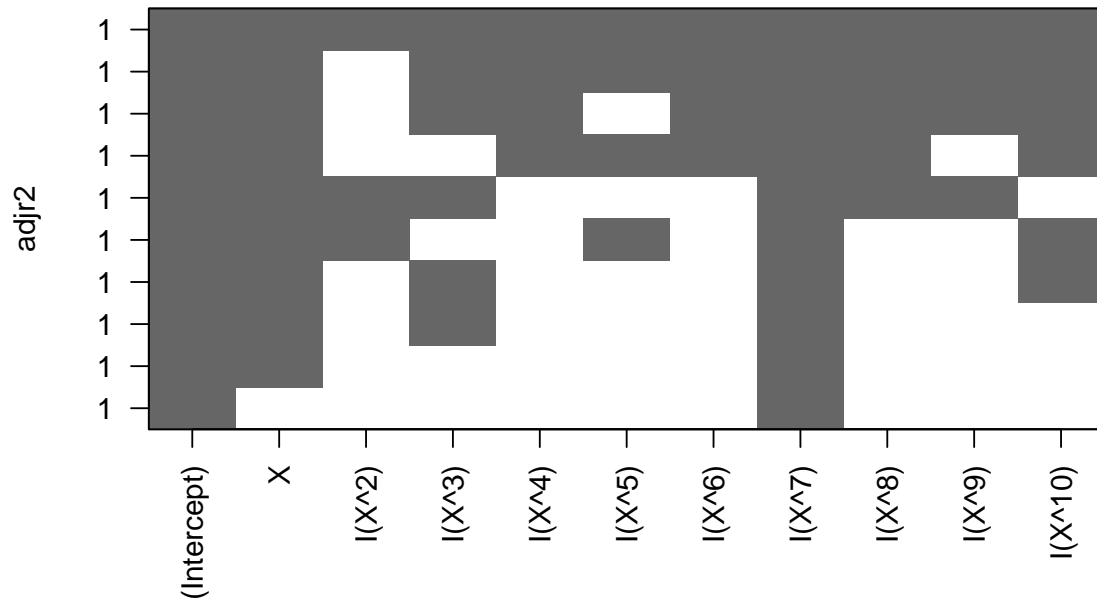
```
plot(mse_v)
title(c("$Y=\beta_0+ \beta_1 X^7$ MSE versus model size for forward subset selection algorithm on train",
"Best SSS"))
```

**+  $\beta_1 X^7$  MSE versus model size for forward subset selection algorithm  
Best SSS**



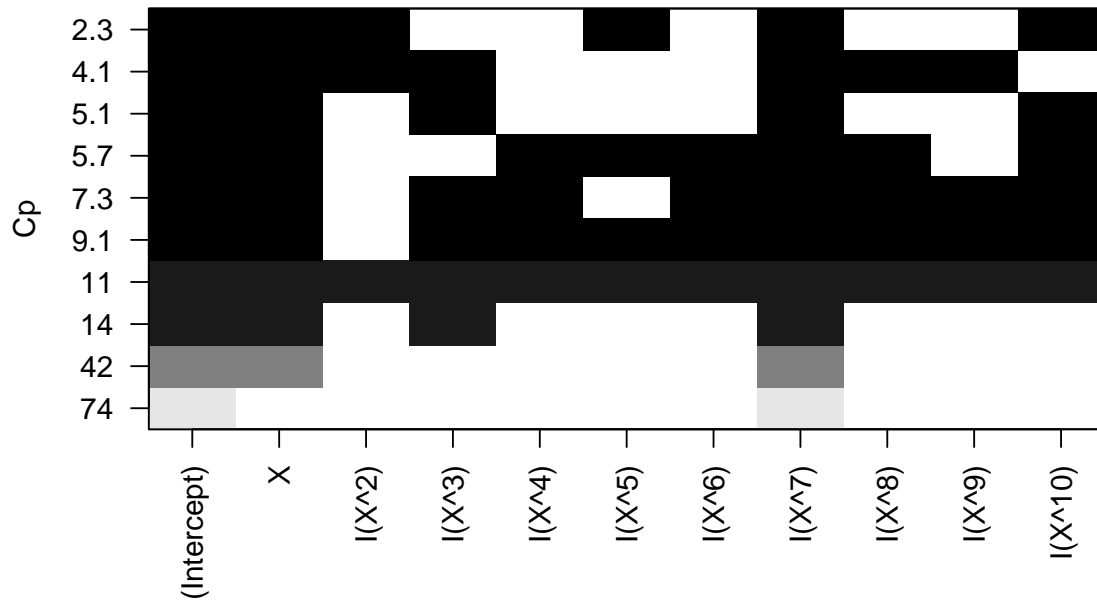
```
plot(regfit.full, scale = "adjr2")
title("Adjuster  $R^2$  statistic Best SSS")
```

### Adjuster $R^2$ statistic Best SSS



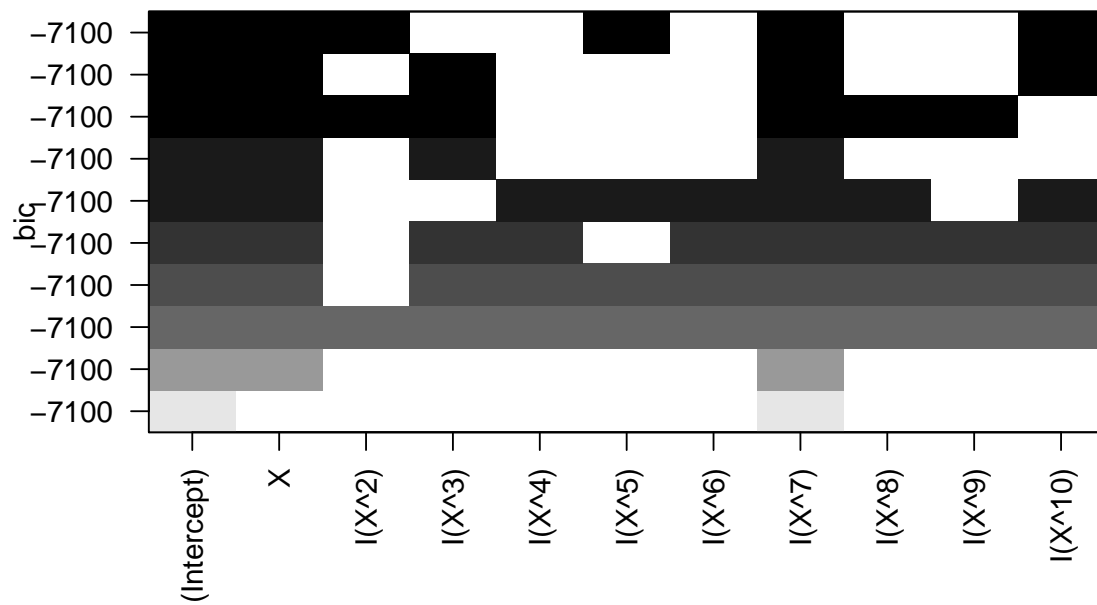
```
plot(regfit.full, scale = "Cp")
title("$Y=\beta_0+ \beta_1 X^7$ Mallow $C_p$ Best SSS")
```

$Y = \eta_0 + \eta_1 X^7$  Mallow  $C_p$  Best SSS

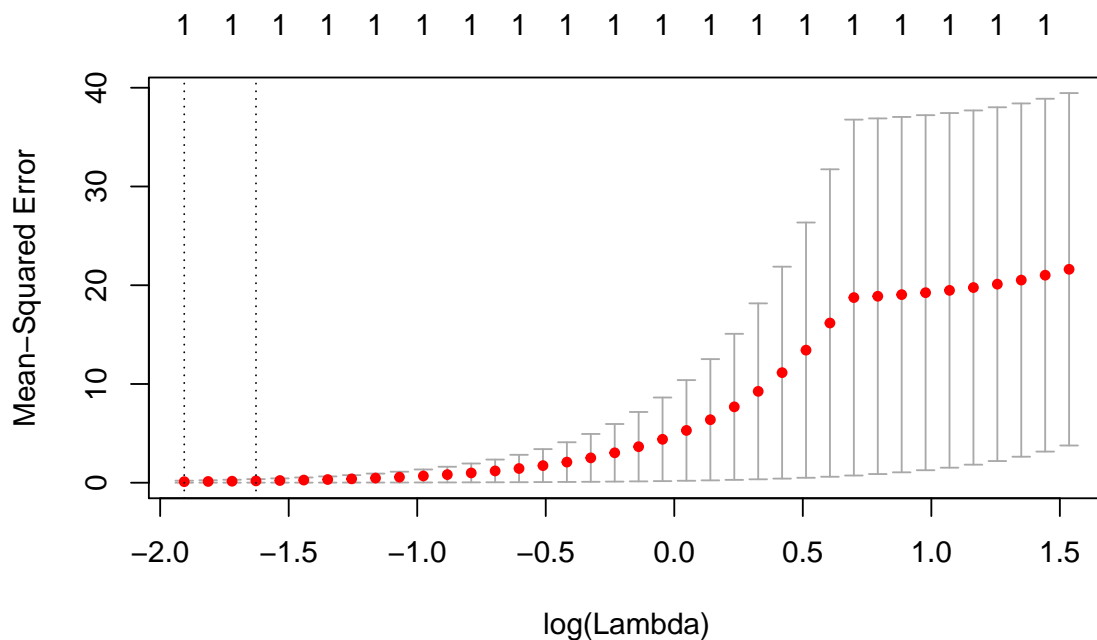


```
plot(regfit.full, scale = "bic")
title("$Y=\\beta_0+ \\beta_1 X^7$ BIC Best SSS")
```

$Y = \eta_0 + \eta_1 X^7$  BIC Best SSS



```
x_lasso = model.matrix(Y ~ 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^10), DF)[, -1]
y_lasso = DF$Y
cv.out = cv.glmnet(x_lasso, y_lasso, alpha = 1)
plot(cv.out)
```



```
bestlam = cv.out$lambda.min
bestlam
```

```
## [1] 0.1486221
```

```
best_lasso = glmnet(x_lasso, y_lasso, alpha = 1, lambda = bestlam)
predict(best_lasso, type = "coefficients", s = bestlam)[1:10, ]
```

```
##      (Intercept)          X      I(X^2)      I(X^3)      I(X^4)
## 1.590678e+00  0.000000e+00  0.000000e+00  0.000000e+00  0.000000e+00
##      I(X^5)      I(X^6)      I(X^7)      I(X^8)      I(X^9)
## 0.000000e+00  0.000000e+00 -8.557615e-02  0.000000e+00 -2.777786e-05
```

All subset selection methods select the 7th term, but none have just that term and the intercept. The adjusted RSS statistic is confused, we suspect because the coefficient for  $X^7$  (randomly generated) was small. The other statistics for Best subset models include additional terms. The lasso with a regularization parameter chose by cross validation comes very close to correctly selecting the model  $Y = \beta_0 + \beta_1 X^7$ . There is a  $X^9$  term with a very small coefficient.

We note that this model may be difficult to fit since the range of the predictor is close to  $[-1, 1]$  where a high order term like  $x^7$  is relatively constant.