Statistical methods for bioinformatics
Model selection and regularization

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1 Conceptual exercises

1.1 Question 5

1.1.1 Part a

We want to minimize the ridge regression defined by $RSS + \lambda \sum_{i=1}^{p} \hat{\beta}_i^2$

- $min\Big[\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \sum_{j=1}^{p}\hat{\beta}_j x_j)^2 + \lambda \sum_{i=1}^{p}\hat{\beta}_i^2\Big]$
- we have as constraints that $\hat{\beta}_0 = 0, p = 2$, hence we can reformulate the optimisation as $min\Big[\sum_{i=1}^{n}(y_i - \sum_{j=1}^{2}\hat{\beta}_j x_j)^2 + \lambda \sum_{i=1}^{2}\hat{\beta}_i^2\Big]$
- which can be expanded into $min\Big[(y_1 - \hat{\beta}_1 x_{11} - \hat{\beta}_2 x_{12})^2 + (y_2 - \hat{\beta}_1 x_{21} - \hat{\beta}_2 x_{22})^2 + \lambda(\hat{\beta}_1^2 + \hat{\beta}_2^2)\Big]$

1.1.2 Part b

For this, we can simply take the derivatives of the ridge regression with respect to $\hat{\beta}_1$ and $\hat{\beta}_2$.

1.1.3 Part c

Very similar to part a, the only difference between the lasso method and the ridge regression lies with the norm taken of the parameters. Lasso used a first-order norm (L1):
$min\Big[(y_1 - \hat{\beta}_1 x_{11} - \hat{\beta}_2 x_{12})^2 + (y_2 - \hat{\beta}_1 x_{21} - \hat{\beta}_2 x_{22})^2 + \lambda(|\hat{\beta}_1| + |\hat{\beta}_2|)\Big]$

1.1.4 Part d

skipped

2 Applied exercises

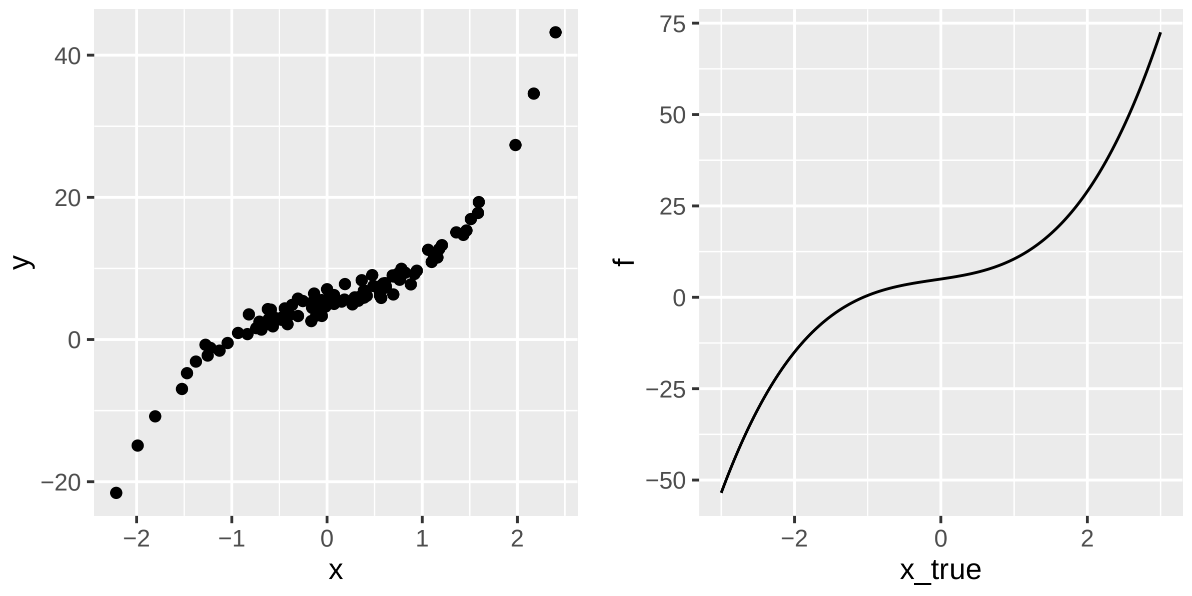
Here is a list of libraries I used for the 2 exercises:

```
library(ggplot2)
library(gridExtra)
library(leaps)
library(glmnet)
options(digits = 2)
```

2.1 Question 8

2.1.1 Part a, b

```
## part a: simulated dataset creation
set.seed(1)
x <- rnorm(100)
noise <- rnorm(100)
x_true <- seq(-3.0,3.0,0.01)

## part b: response vector with given model y = 1x^3 - 2x^2 + 3x + 5
y <- 2*x^3 + 0.5*x^2 + 3*x + 5 + noise
f <- 2*x_true^3 + 0.5*x_true^2 + 3*x_true+ 5

p1 <- qplot(x,y)
p2 <- qplot(x_true,f, geom="line")
grid.arrange(p1, p2, ncol=2)
ggsave("fun.pdf", arrangeGrob(p1, p2, ncol = 2), width = 16, height = 8, units = "cm")
```



2.1.2 Part c

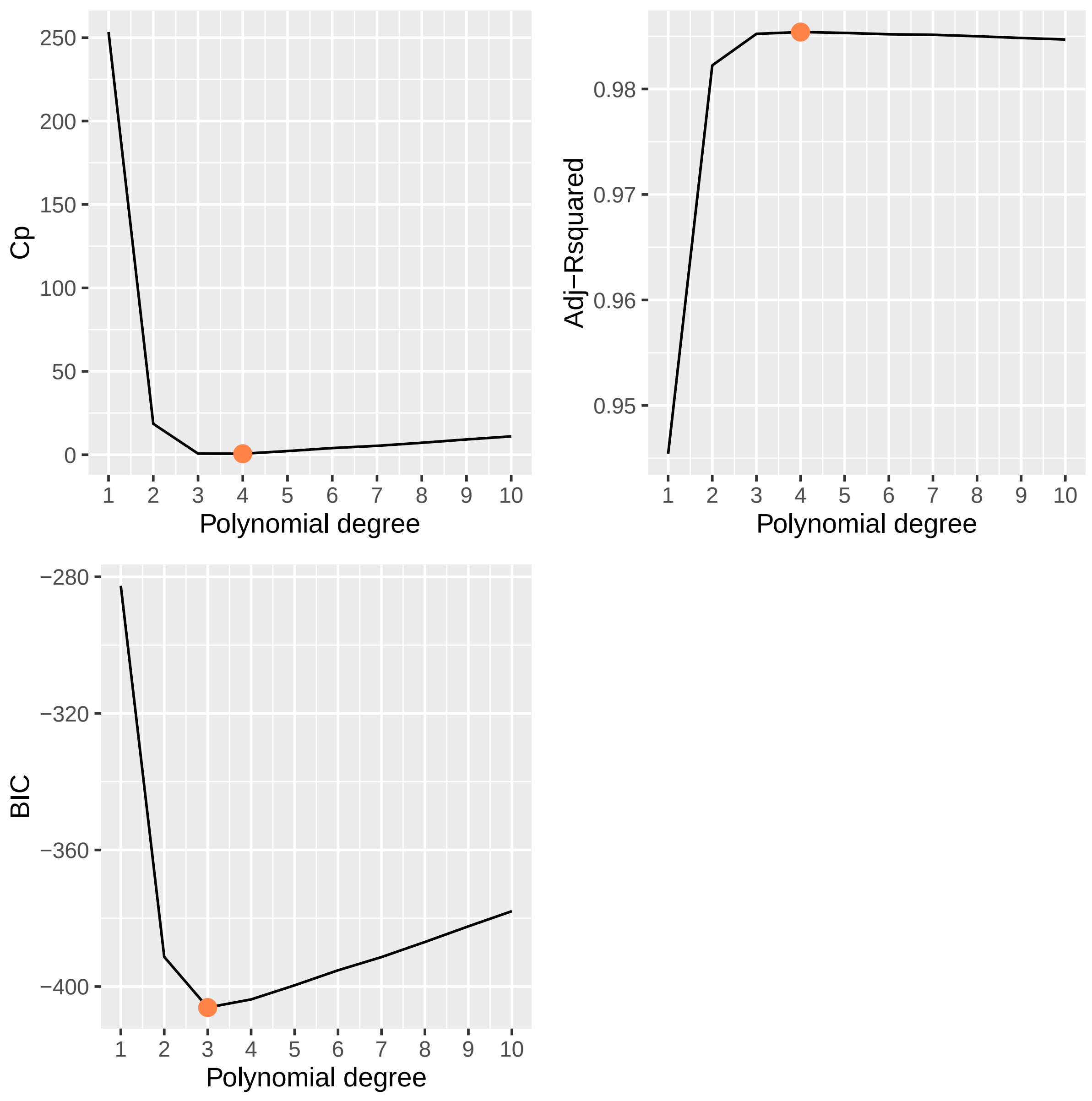
```
## part c: perform best subset selection
dataset <- data.frame(x, y)
```

```r
regfit.full <- regsubsets(y ~ poly(x, 10, raw = TRUE), data = dataset, nvmax = 10)
regfit.summary <- summary(regfit.full)
which.min(regfit.summary$cp)
which.min(regfit.summary$bic)
which.max(regfit.summary$adjr2)

# plotting results
cp <- qplot(1:10, regfit.summary$cp, geom="line") +
    xlab("Polynomial degree") + ylab("Cp") + scale_x_continuous(breaks=seq(1,10,1)) +
    geom_point(aes(x=4,y=regfit.summary$cp[4]),colour=I("sienna1"),size=3)

adjr2 <- qplot(1:10, regfit.summary$adjr2, geom="line") +
    xlab("Polynomial degree") + ylab("Adj-Rsquared") + scale_x_continuous(breaks=seq(1,10,1))
    geom_point(aes(x=4,y=regfit.summary$adjr2[4]),colour=I("sienna1"),size=3)

bic <- qplot(1:10, regfit.summary$bic, geom="line") +
    xlab("Polynomial degree") + ylab("BIC") + scale_x_continuous(breaks=seq(1,10,1)) +
    geom_point(aes(x=3,y=regfit.summary$bic[3]),colour=I("sienna1"),size=3)

grid.arrange(cp, adjr2, bic, ncol=2, nrow=2)
ggsave("BIC-AR2-Cp.pdf", arrangeGrob(cp, adjr2, bic, ncol = 2, nrow=2), )

coefficients(regfit.full, id = 3)
coefficients(regfit.full, id = 4)
```

Here is the summary of the coefficients for the models that include 3 and 4 predictors:

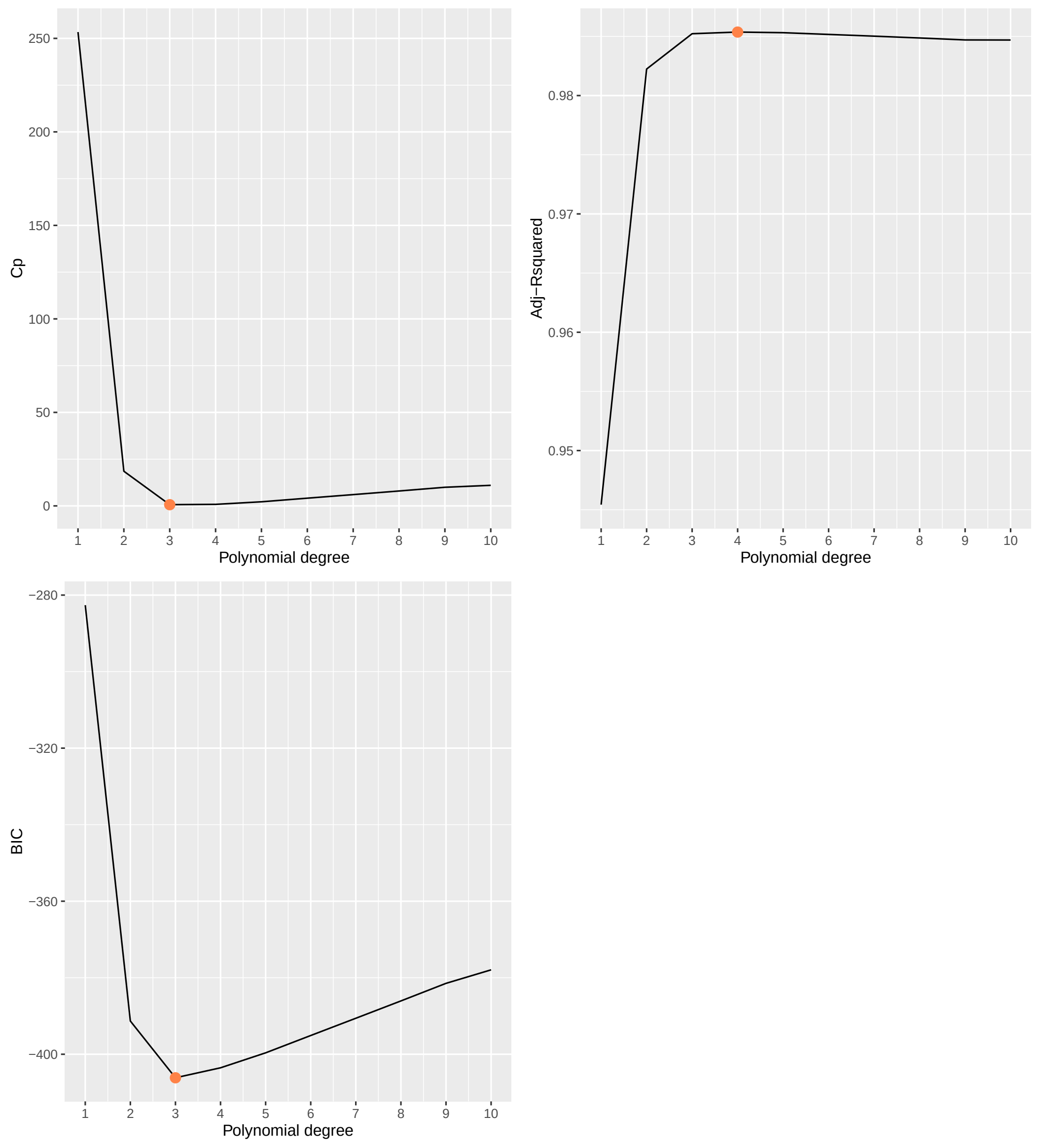
```
> coefficients(regfit.full, id = 3)
          (Intercept) poly(x, 10, raw = T)1 poly(x, 10, raw = T)3
                5.192                 3.043                 1.985
poly(x, 10, raw = T)4
                0.089
> sort(x)  C-c C-c
> coefficients(regfit.full, id = 4)
          (Intercept) poly(x, 10, raw = T)1 poly(x, 10, raw = T)2
                5.072                 3.387                 0.346
poly(x, 10, raw = T)3 poly(x, 10, raw = T)5
                1.558                 0.081
```

The graphs, which upon visual inspection allows to decide which model to use indicate 2 different optimal choices. 3 and 4 predictors. Note that the most convincing graph seems to be the one using the *BIC* criterion. The others have a minimum at 4, but that minimum is very close to that located at 3.



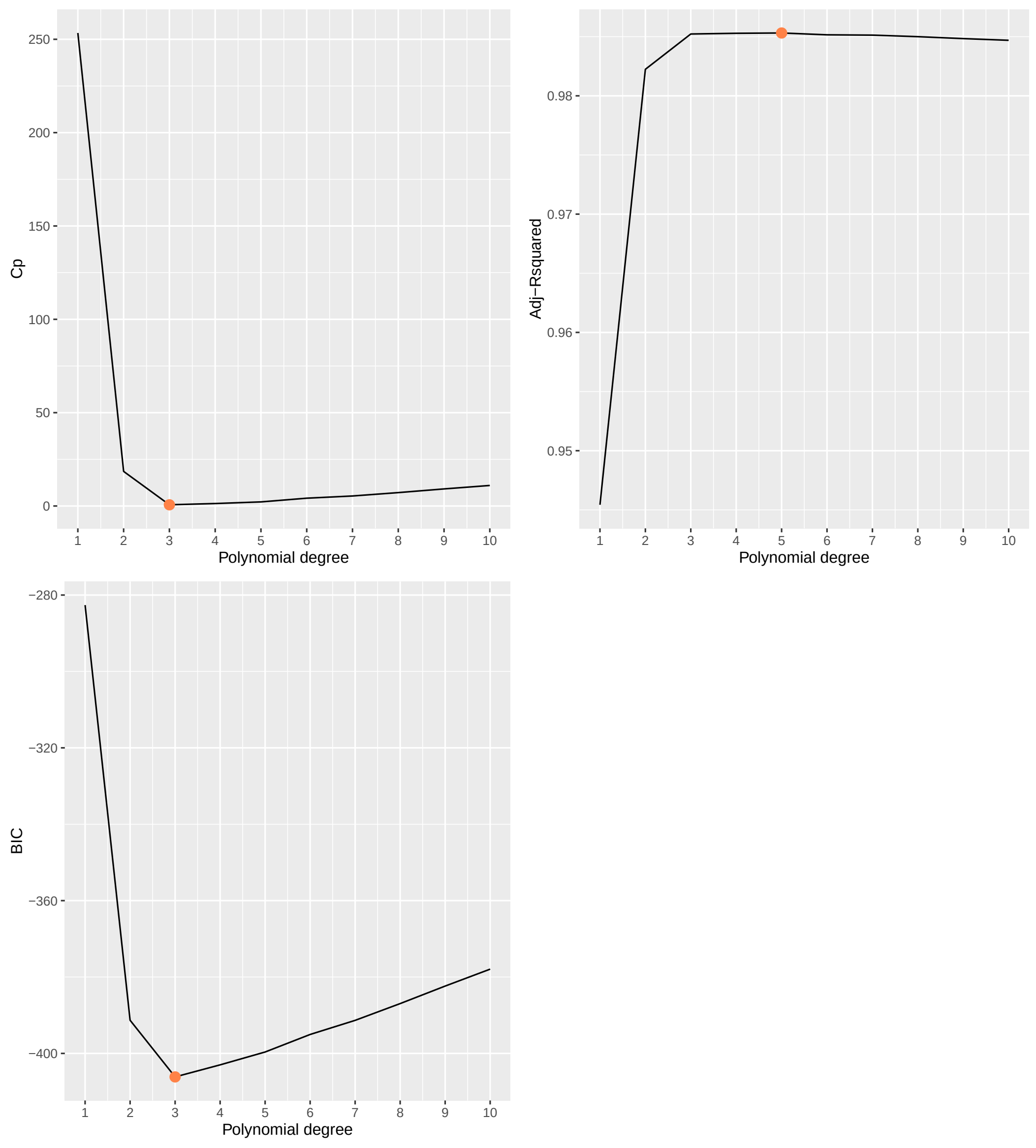
```
## Forward selection
regfit.fwd <- regsubsets(y ~ poly(x, 10, raw = TRUE), data = dataset, nvmax = 10, method = "fo
fwd.summary <-  summary(regfit.fwd)
which.min(fwd.summary$cp)
which.max(fwd.summary$adjr2)
which.min(fwd.summary$bic)

cp <- qplot(1:10, fwd.summary$cp, geom="line") +
    xlab("Polynomial degree") + ylab("Cp") + scale_x_continuous(breaks=seq(1,10,1)) +
    geom_point(aes(x=3,y=fwd.summary$cp[3]),colour=I("sienna1"),size=3)

adjr2 <- qplot(1:10, fwd.summary$adjr2, geom="line") +
    xlab("Polynomial degree") + ylab("Adj-Rsquared") + scale_x_continuous(breaks=seq(1,10,1))
    geom_point(aes(x=4,y=fwd.summary$adjr2[4]),colour=I("sienna1"),size=3)
```

```
bic <- qplot(1:10, fwd.summary$bic, geom="line") +
    xlab("Polynomial degree") + ylab("BIC") + scale_x_continuous(breaks=seq(1,10,1)) +
    geom_point(aes(x=3,y=fwd.summary$bic[3]),colour=I("sienna1"),size=3)

grid.arrange(cp, adjr2, bic, ncol=2, nrow=2)
ggsave("Fwd-BIC-AR2-Cp.pdf", arrangeGrob(cp, adjr2, bic, ncol = 2, nrow=2))
```



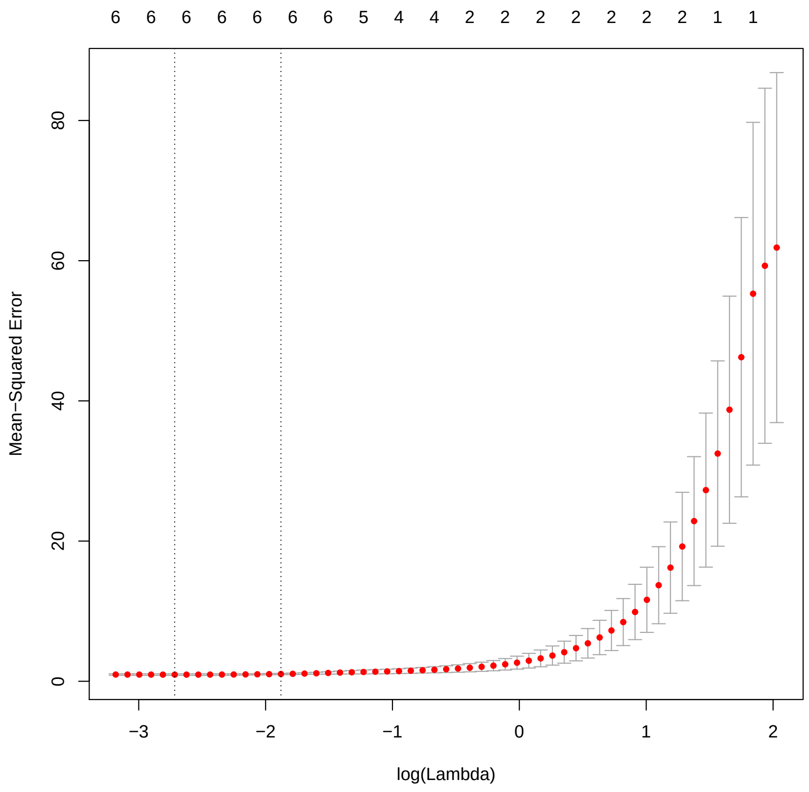
2.1.3 Part d

```
## Backward selection
regfit.bwd <- regsubsets(y ~ poly(x, 10, raw = TRUE), data = dataset, nvmax = 10, method = "ba
bwd.summary <-  summary(regfit.bwd)

which.min(bwd.summary$cp)
which.max(bwd.summary$adjr2)
which.min(bwd.summary$bic)

cp <- qplot(1:10, bwd.summary$cp, geom="line") +
    xlab("Polynomial degree") + ylab("Cp") + scale_x_continuous(breaks=seq(1,10,1)) +
    geom_point(aes(x=3,y=bwd.summary$cp[3]),colour=I("sienna1"),size=3)

adjr2 <- qplot(1:10, bwd.summary$adjr2, geom="line") +
    xlab("Polynomial degree") + ylab("Adj-Rsquared") + scale_x_continuous(breaks=seq(1,10,1))
    geom_point(aes(x=5,y=bwd.summary$adjr2[5]),colour=I("sienna1"),size=3)

bic <- qplot(1:10, bwd.summary$bic, geom="line") +
    xlab("Polynomial degree") + ylab("BIC") + scale_x_continuous(breaks=seq(1,10,1)) +
    geom_point(aes(x=3,y=bwd.summary$bic[3]),colour=I("sienna1"),size=3)

grid.arrange(cp, adjr2, bic, ncol=2, nrow=2)
ggsave("Bwd-BIC-AR2-Cp.pdf", arrangeGrob(cp, adjr2, bic, ncol = 2, nrow=2))
```



2.1.4 Part e

```
xmat <- model.matrix(y ~ poly(x, 10, raw = T), data = dataset)[, -1]
lasso.mod <- cv.glmnet(xmat, y, alpha = 1)
best.lambda <- lasso.mod$lambda.min

pdf("lasso-plot.pdf", width=8, height=8)
plot(lasso.mod)
dev.off()

# Next fit the model on entire data using best lambda
best.model <- glmnet(xmat, y, alpha = 1)
predict(best.model, s = best.lambda, type = "coefficients")
```



```
> predict(best.model, s = best.lambda, type = "coefficients")
11 x 1 sparse Matrix of class "dgCMatrix"
                              1
(Intercept)              5.1776
poly(x, 10, raw = T)1   3.1552
poly(x, 10, raw = T)2   0.1273
poly(x, 10, raw = T)3   1.8183
poly(x, 10, raw = T)4   0.0422
poly(x, 10, raw = T)5   0.0032
poly(x, 10, raw = T)6   .
poly(x, 10, raw = T)7   0.0054
poly(x, 10, raw = T)8  .
poly(x, 10, raw = T)9  .
poly(x, 10, raw = T)10 .
```

2.1.5 Part f

For this exercise, I used the following underlying function, with Gaussian noise:

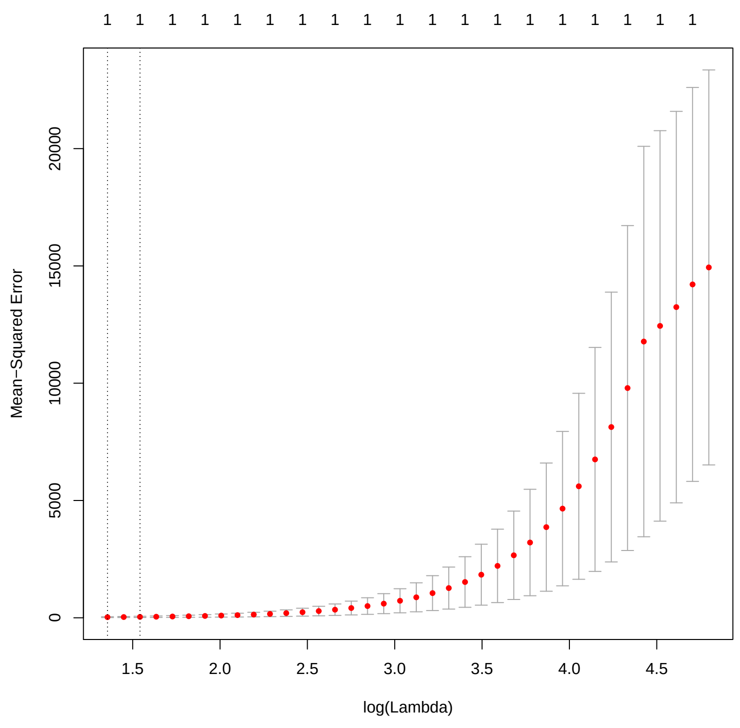
```
y <- 5 + 2*x^7 + noise
dataset <- data.frame(x, y)
```

Here is the best subset approach:

```
## Best subset
regfit.full <- regsubsets(y ~ poly(x, 10, raw = TRUE), data = dataset, nvmax = 10)
regfit.summary <- summary(regfit.full)
which.min(regfit.summary$cp)
which.min(regfit.summary$bic)
which.max(regfit.summary$adjr2)

# plotting results best subset
cp <- qplot(1:10, regfit.summary$cp, geom="line") +
    xlab("Polynomial degree") + ylab("Cp") + scale_x_continuous(breaks=seq(1,10,1)) +
    geom_point(aes(x=2,y=regfit.summary$cp[2]),colour=I("sienna1"),size=3)

adjr2 <- qplot(1:10, regfit.summary$adjr2, geom="line") +
    xlab("Polynomial degree") + ylab("Adj-Rsquared") + scale_x_continuous(breaks=seq(1,10,1))
    geom_point(aes(x=4,y=regfit.summary$adjr2[4]),colour=I("sienna1"),size=3)

bic <- qplot(1:10, regfit.summary$bic, geom="line") +
    xlab("Polynomial degree") + ylab("BIC") + scale_x_continuous(breaks=seq(1,10,1)) +
    geom_point(aes(x=1,y=regfit.summary$bic[1]),colour=I("sienna1"),size=3)

grid.arrange(cp, adjr2, bic, ncol=2, nrow=2)
ggsave("BIC-AR2-Cp-f.pdf", arrangeGrob(cp, adjr2, bic, ncol = 2, nrow=2),
       width = 16, height = 16, units = "cm")
```

And the lasso approach:

```
## Lasso
xmat <- model.matrix(y ~ poly(x, 10, raw = T), data = dataset)[, -1]
lasso.mod <- cv.glmnet(xmat, y, alpha = 1)
best.lambda <- lasso.mod$lambda.min

best.model <- glmnet(xmat, y, alpha = 1)
predict(best.model, s = best.lambda, type = "coefficients")

pdf("lasso-plot-f.pdf", width=8, height=8)
plot(lasso.mod)
dev.off()
```



As shown below for the coefficients, the lasso model is really spot on when considering the underlying model used to generate the dataset.

```
> predict(best.model, s = best.lambda, type = "coefficients")
11 x 1 sparse Matrix of class "dgCMatrix"
                          1
(Intercept)             5.2
poly(x, 10, raw = T)1   .
poly(x, 10, raw = T)2   .
poly(x, 10, raw = T)3   .
poly(x, 10, raw = T)4   .
poly(x, 10, raw = T)5   .
poly(x, 10, raw = T)6   .
poly(x, 10, raw = T)7   1.9
poly(x, 10, raw = T)8   .
poly(x, 10, raw = T)9   .
poly(x, 10, raw = T)10 .
```