HW3

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Question 4 (ISL Chapter 7, Exercise 9)

This question uses the variables dis (the weighted mean of distances to five Boston employment centers) and nox (nitrogen oxides concentration in parts per 10 million) from the Boston data. We will treat dis as the predictor and nox as the response.

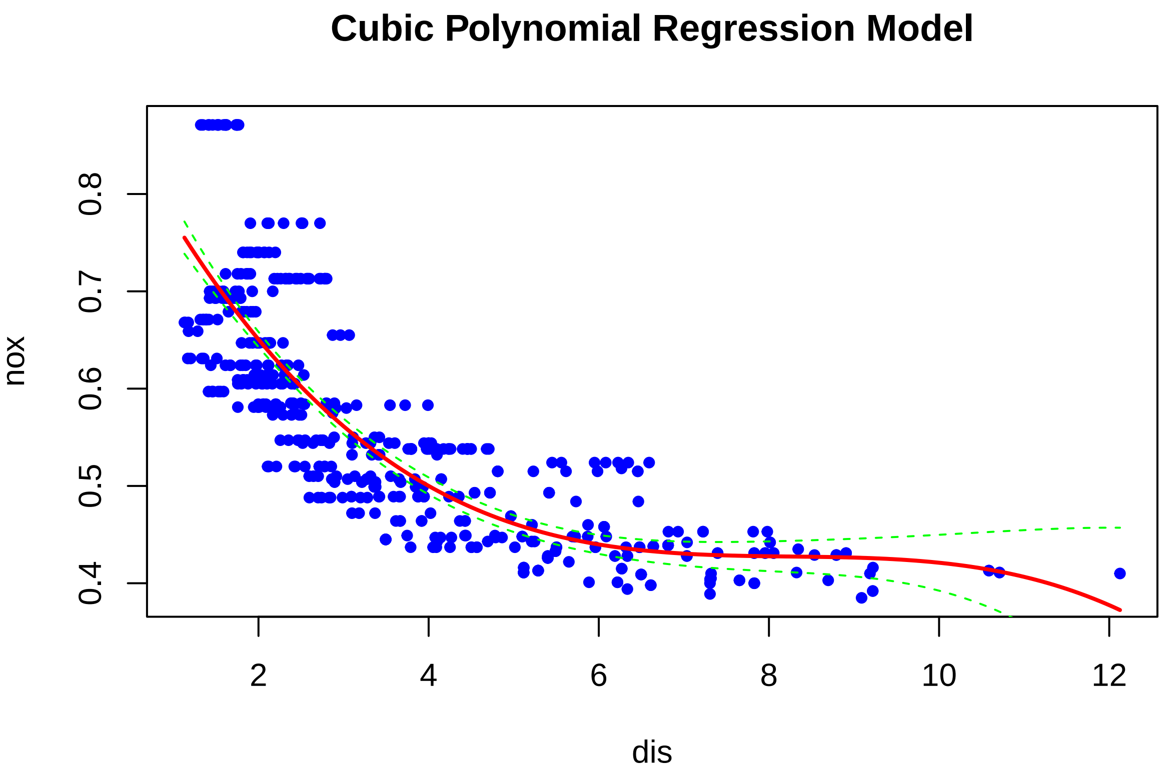
```
library(MASS)
library(boot)
library(splines)
data("Boston")
attach(Boston)
```

a. Use the poly() function to fit a cubic polynomial regression to predict nox using dis. Report the regression output, and plot the resulting data and polynomial fits.

```
# Fit cubic polynomial regression model
cubic_model <- lm(nox ~ poly(dis, 3))
summary(cubic_model)
```

```
##
## Call:
## lm(formula = nox ~ poly(dis, 3))
##
## Residuals:
##       Min        1Q    Median        3Q       Max
## -0.121130 -0.040619 -0.009738  0.023385  0.194904
##
## Coefficients:
##                Estimate Std. Error t value Pr(>|t|)
## (Intercept)    0.554695   0.002759 201.021  < 2e-16 ***
## poly(dis, 3)1 -2.003096   0.062071 -32.271  < 2e-16 ***
## poly(dis, 3)2  0.856330   0.062071  13.796  < 2e-16 ***
## poly(dis, 3)3 -0.318049   0.062071  -5.124 4.27e-07 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.06207 on 502 degrees of freedom
## Multiple R-squared:  0.7148, Adjusted R-squared:  0.7131
## F-statistic: 419.3 on 3 and 502 DF,  p-value: < 2.2e-16
```

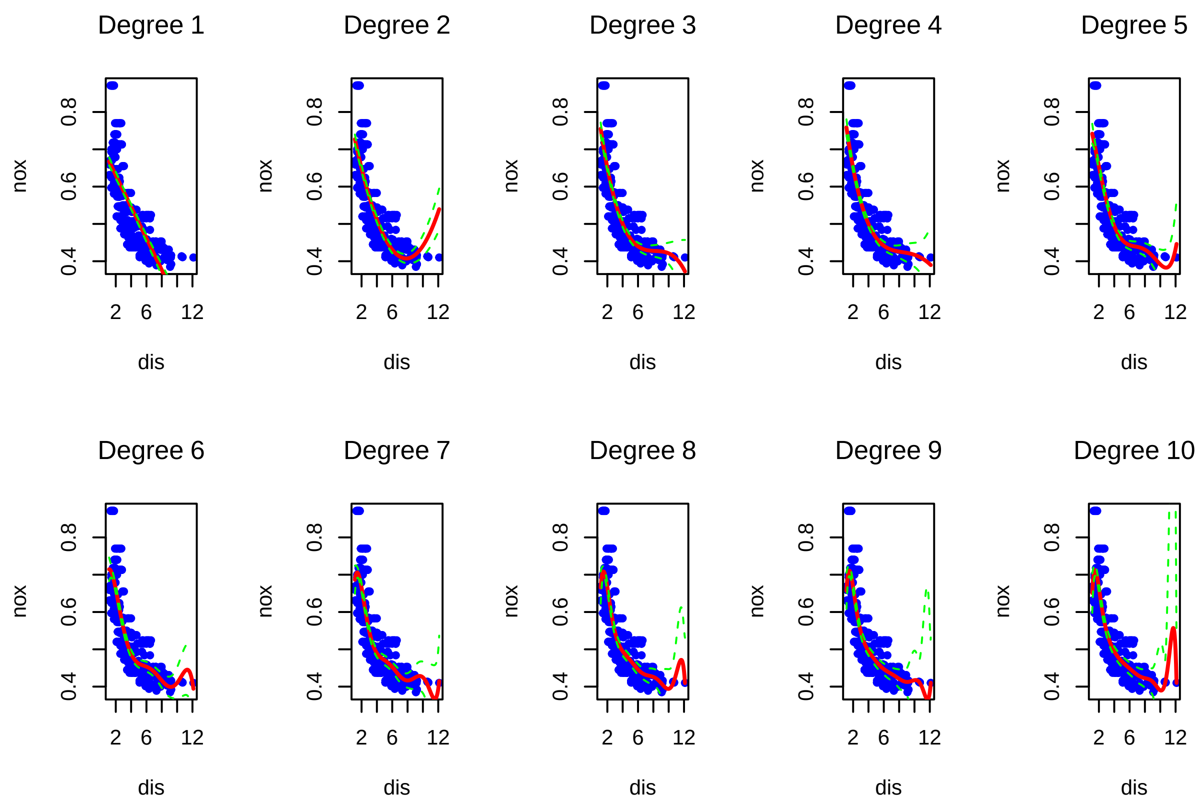
```r
# Plot
dis_seq <- seq(min(dis), max(dis), length.out = nrow(Boston))

predictions <- predict(cubic_model,
                       newdata = data.frame(dis = dis_seq),
                       se.fit = TRUE)

predicted_nox <- predictions$fit
se <- predictions$se.fit

plot(dis, nox, pch = 20, col = "blue")
lines(dis_seq, predicted_nox, col = "red", lwd = 2)
lines(dis_seq, predicted_nox + 2 * se, col = "green", lty = 2)
lines(dis_seq, predicted_nox - 2 * se, col = "green", lty = 2)
title("Cubic Polynomial Regression Model")
```



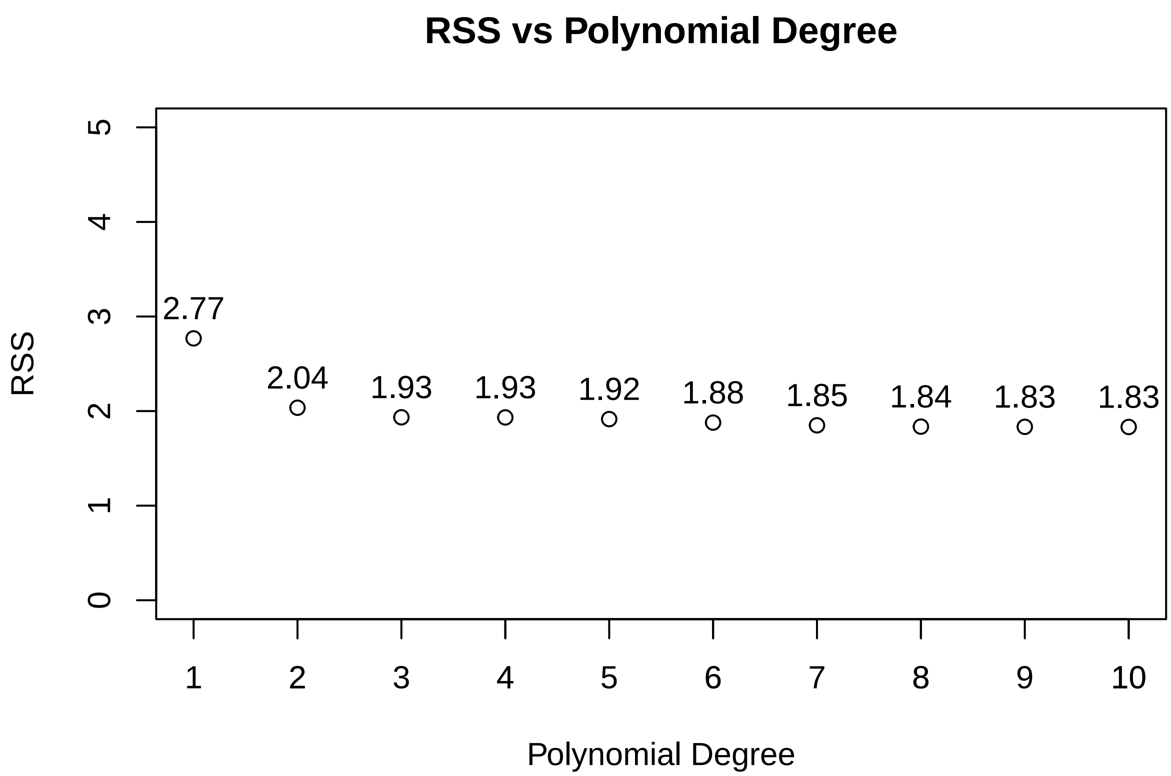
(b) Plot the polynomial fits for a range of different polynomial degrees (say, from 1 to 10), and report the associated residual sum of squares.

```r
# Fit degree 1-10 models and plot
par(mfrow = c(2, 5))
rss_vals <- numeric(10)
for (i in 1:10){
  model <- lm(nox ~ poly(dis, i))

  dis_seq <- seq(min(dis), max(dis), length.out = nrow(Boston))

  predictions <- predict(model,
```

```
                                newdata = data.frame(dis = dis_seq),
                                se.fit = TRUE)

  predicted_nox <- predictions$fit
  se <- predictions$se.fit

  plot(dis, nox, pch = 20, col = "blue",
       main = bquote("Degree" ~ .(i)))
  lines(dis_seq, predicted_nox, col = "red", lwd = 2)
  lines(dis_seq, predicted_nox + 2 * se, col = "green", lty = 2)
  lines(dis_seq, predicted_nox - 2 * se, col = "green", lty = 2)

  rss_vals[i] = sum(model$residuals^2)
}
```




```
# Plot RSS
plot(rss_vals,
     xlab = "Polynomial Degree",
     ylab = "RSS",
     main = "RSS vs Polynomial Degree",
     ylim = c(0, 5))
axis(1, at = 1:10, labels = 1:10)
text(1:10, rss_vals, labels = round(rss_vals, digits = 2), pos = 3)
```



The above graph shows the RSS values for polynomial degree 1-10.

(c) Perform cross-validation or another approach to select the optimal degree for the polynomial, and explain your results.

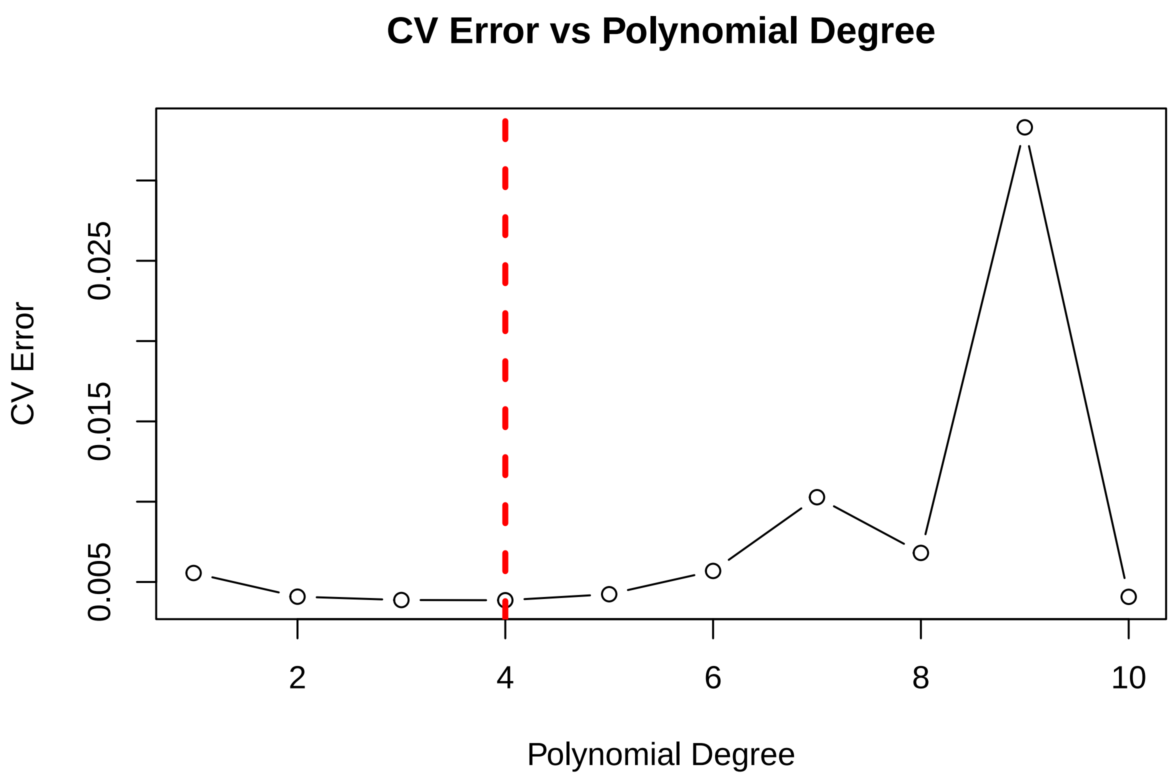
```
# Perform CV
set.seed(1)
cv.error <- numeric(10)
for (i in 1:10){
  fit = glm(nox ~ poly(dis,i))
  cv.error[i] = cv.glm(Boston,fit, K =10)$delta[1]
}

print(cv.error)
```

```
##  [1] 0.005558263 0.004085706 0.003876521 0.003863342 0.004237452 0.005686862
##  [7] 0.010278897 0.006810868 0.033308607 0.004075599
```

```
best_degree <- which.min(cv.error)
cat("The degree with the smallest cross-validation error is", best_degree)
```

```
## The degree with the smallest cross-validation error is 4
```

```
# Plot CV
plot(cv.error,
     type = "b",
     xlab = "Polynomial Degree",
     ylab = "CV Error",
     main = "CV Error vs Polynomial Degree")
abline(v = 4, col = "red", lwd = 3, lty = 2)
```



We performed 10-fold cross validation and computed the validation error for different polynomial degrees (1-10). The degree that yielded the minimum CV error is degree 4, which had an error of 0.003863342, and this implies degree 4 might be the optimal degree for this question, but test MSPE needs to be assessed to prove it.

(d) Use the bs() function to fit a regression spline to predict nox using dis. Report the output for the fit using four degrees of freedom. How did you choose the knots? Plot the resulting fit.

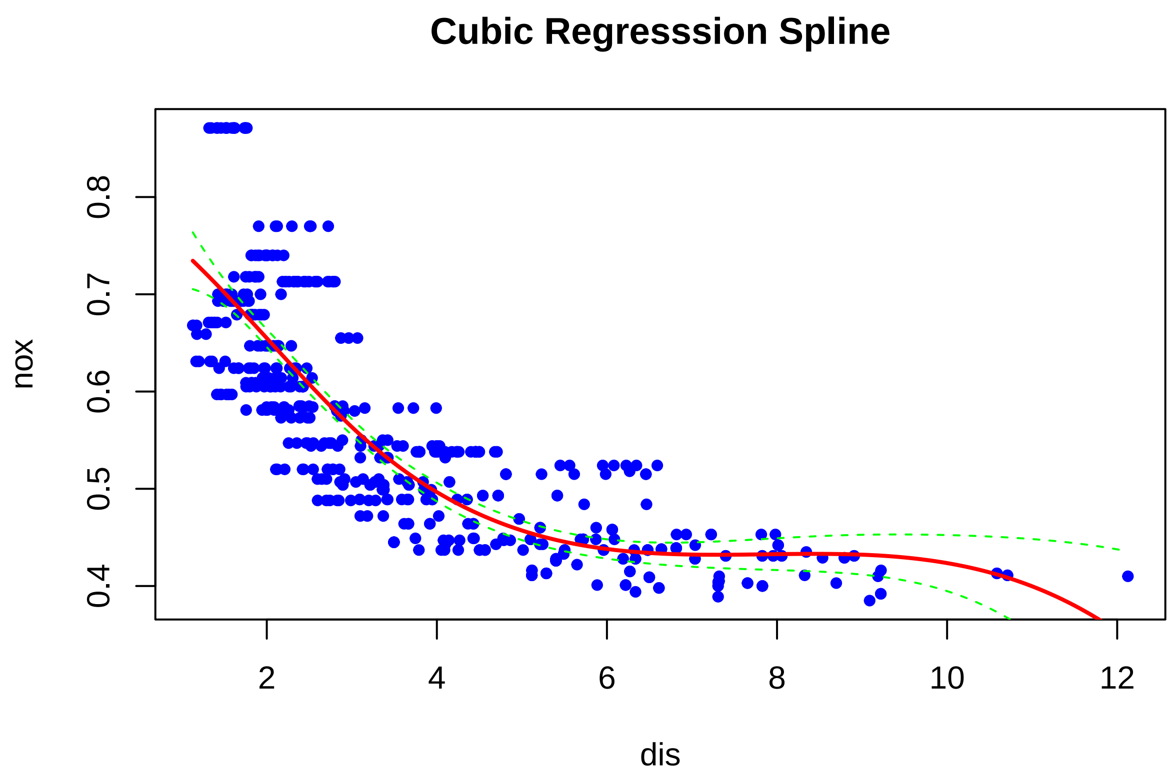
To choose the knots, we know that cubic spline with K knots would have K + 4 parameters or degrees of freedom. Therefore, with four degrees of freedom we can only have a cubic spline with zero knot.

```r
# Fit cubic spline
cs.fit <- lm(nox ~ bs(dis, df = 4))
summary(cs.fit)
```

```
##
## Call:
## lm(formula = nox ~ bs(dis, df = 4))
##
## Residuals:
##       Min        1Q    Median        3Q       Max
## -0.124622 -0.039259 -0.008514  0.020850  0.193891
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)        0.73447    0.01460  50.306  < 2e-16 ***
## bs(dis, df = 4)1 -0.05810    0.02186  -2.658  0.00812 **
## bs(dis, df = 4)2 -0.46356    0.02366 -19.596  < 2e-16 ***
## bs(dis, df = 4)3 -0.19979    0.04311  -4.634 4.58e-06 ***
## bs(dis, df = 4)4 -0.38881    0.04551  -8.544  < 2e-16 ***
## ---
```

```
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.06195 on 501 degrees of freedom
## Multiple R-squared:  0.7164, Adjusted R-squared:  0.7142
## F-statistic: 316.5 on 4 and 501 DF,  p-value: < 2.2e-16
```

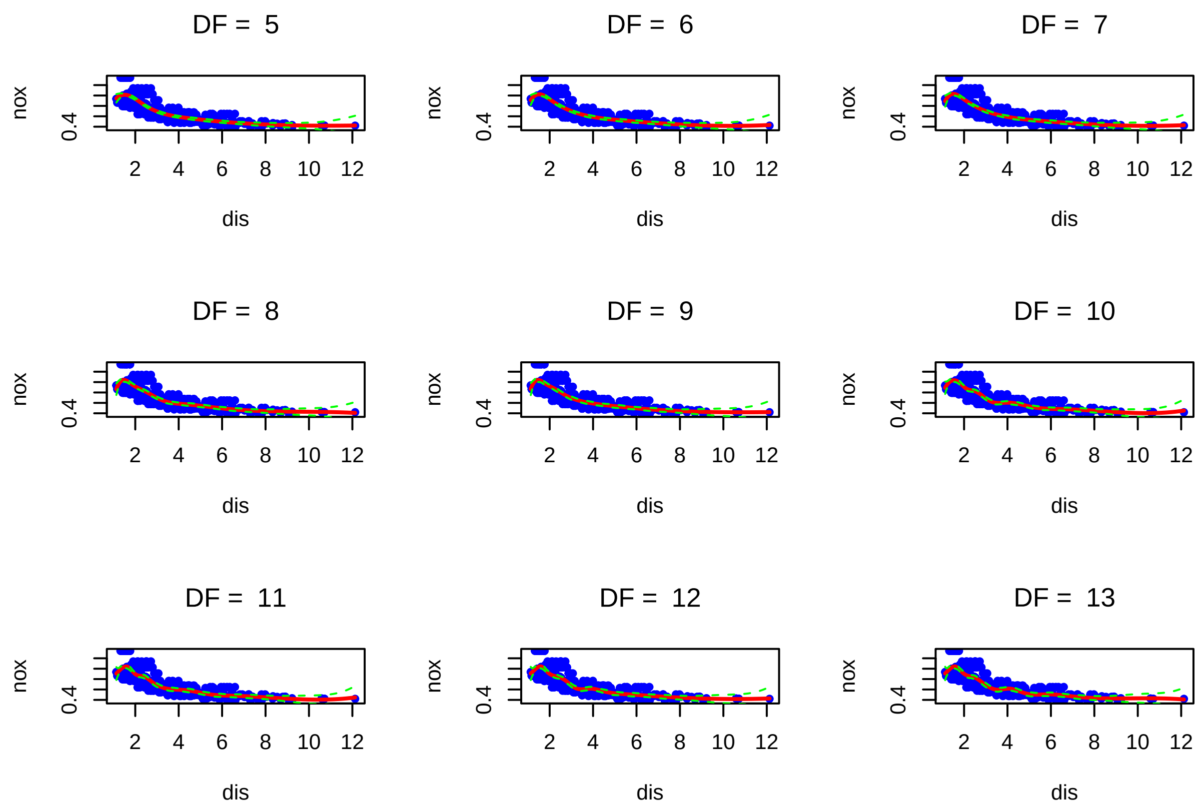
```
# Plot
dis_seq <- seq(min(dis), max(dis), length.out = nrow(Boston))

predictions <- predict(cs.fit,
                       newdata = data.frame(dis = dis_seq),
                       se.fit = TRUE)

predicted_nox <- predictions$fit
se <- predictions$se.fit

plot(dis, nox, pch = 20, col = "blue")
lines(dis_seq, predicted_nox, col = "red", lwd = 2)
lines(dis_seq, predicted_nox + 2 * se, col = "green", lty = 2)
lines(dis_seq, predicted_nox - 2 * se, col = "green", lty = 2)
title("Cubic Regresssion Spline")
```



(e) Now fit a regression spline for a range of degrees of freedom, and plot the resulting fits and report the resulting RSS. Describe the results obtained.

```
# Fit df 5-13 splines and plot
par(mfrow = c(3, 3))
rss_vals <- numeric(9)
for (i in 5:13){
```

```
  cs.fit <- lm(nox ~ bs(dis, df = i))

  dis_seq <- seq(min(dis), max(dis), length.out = nrow(Boston))

  predictions <- predict(cs.fit,
                         newdata = data.frame(dis = dis_seq),
                         se.fit = TRUE)

  predicted_nox <- predictions$fit
  se <- predictions$se.fit

  plot(dis, nox, pch = 20, col = "blue",
       main = bquote("DF = " ~ .(i)))
  lines(dis_seq, predicted_nox, col = "red", lwd = 2)
  lines(dis_seq, predicted_nox + 2 * se, col = "green", lty = 2)
  lines(dis_seq, predicted_nox - 2 * se, col = "green", lty = 2)

  rss_vals[i-4] = sum(cs.fit$residuals^2)
}
```



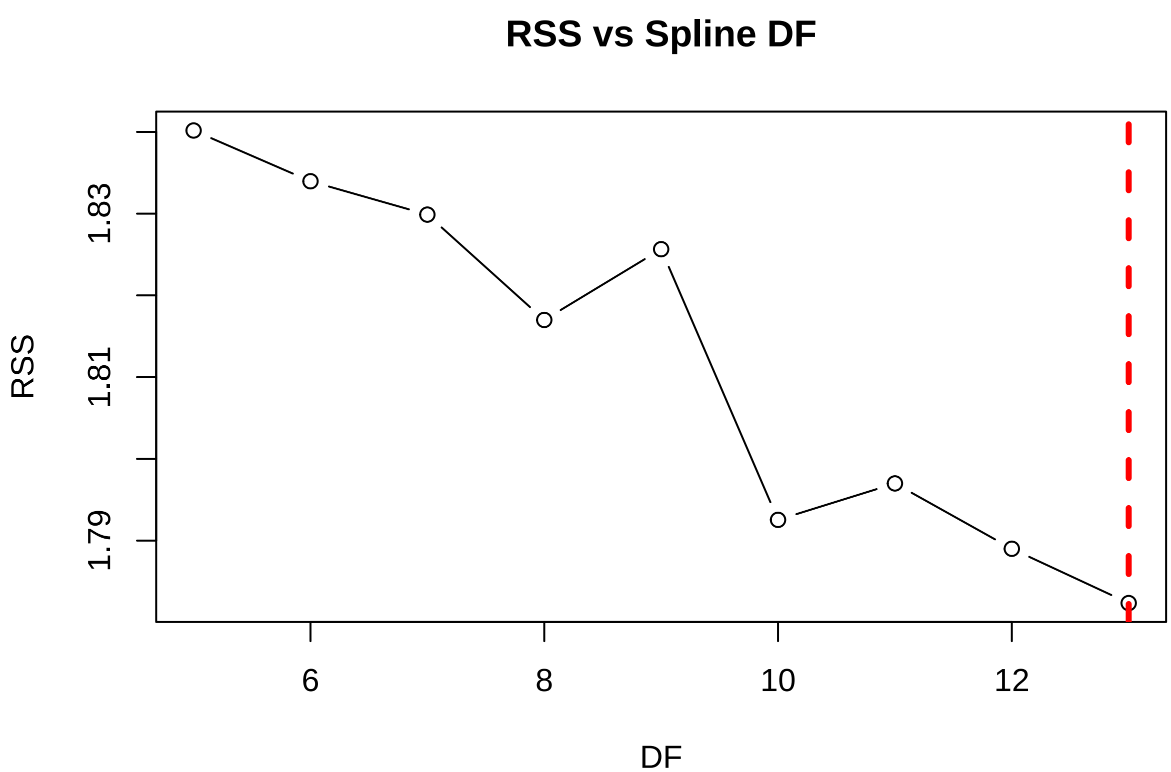

```
print(rss_vals)
```

```
## [1] 1.840173 1.833966 1.829884 1.816995 1.825653 1.792535 1.796992 1.788999
## [9] 1.782350
```

```r
best_df <- which.min(rss_vals) + 4
cat("The df with the smallest RSS is", best_df)
```

```
## The df with the smallest RSS is 13
```

```r
# Plot RSS
degrees_of_freedom <- 5:13
plot(degrees_of_freedom, rss_vals,
     type = "b",
     xlab = "DF",
     ylab = "RSS",
     main = "RSS vs Spline DF")
abline(v = 13, col = "red", lwd = 3, lty = 2)
```



We tried degree of freedom 5-13 for the cubic splines and computed the RSS for each. The DF that yielded the minimum RSS is 13 (the largest we tried), which had an error of 1.782350. For cubic spline models with higher degrees of freedom (more knots), the model generally has less RSS. However, they are generally more wiggly than models with fewer degrees of freedom. This illustrates the bias-variance tradeoff — more complex & flexible models (cubic splines with higher degrees of freedom) have lower bias (lower RSS) but higher variance, and vice versa.

(f) Perform cross-validation or another approach in order to select the best degrees of freedom for a regression spline on this data. Describe your results.

```r
# Perform CV
set.seed(1)
cv.error <- numeric(9)
for (i in 5:13){
  fit <- glm(nox ~ bs(dis, df = i))
```

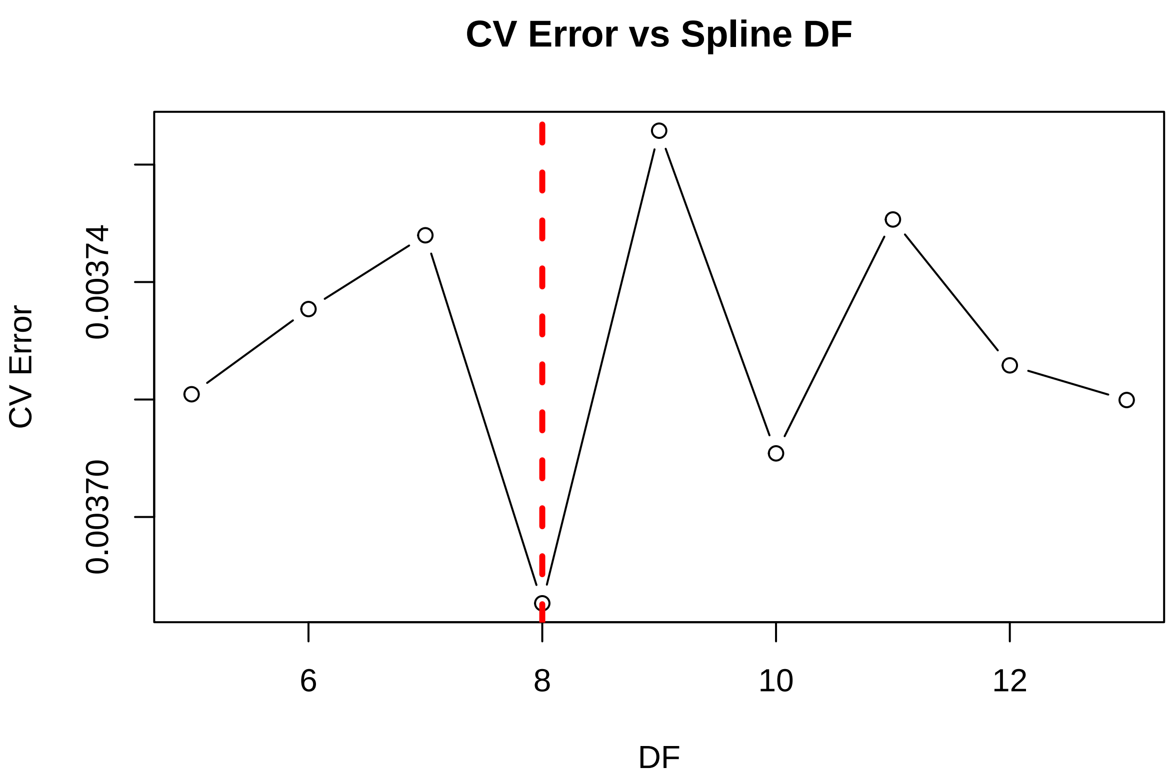
```r
  cv.error[i-4] = cv.glm(Boston,fit, K = 10)$delta[1]
}

print(cv.error)
```

```
## [1] 0.003720901 0.003735400 0.003747967 0.003685305 0.003765768 0.003710831
## [7] 0.003750657 0.003725816 0.003719913
```

```r
best_degree <- which.min(cv.error) + 4
cat("The df with the smallest cross-validation error is", best_degree)
```

```
## The df with the smallest cross-validation error is 8
```

```r
# Plot CV
degrees_of_freedom <- 5:13
plot(degrees_of_freedom, cv.error,
     type = "b",
     xlab = "DF",
     ylab = "CV Error",
     main = "CV Error vs Spline DF")
abline(v = 8, col = "red", lwd = 3, lty = 2)
```



We performed 10-fold cross validation and computed the validation error for different degrees of freedom (5-13) for the cubic splines. The df that yielded the minimum CV error is 8, which had an error of 0.003685305, and this implies `df = 8` might be the optimal df for this question, but test MSPE needs to be assessed to prove it. Also, a caveat is that the difference in CV errors for these df's being examined is actually very small, and we know that complex models might be harder to interpret. Therefore, in reality, model with smaller df might be chosen.