STATS 790 Assignment 3

Yiran Zhang
400119421

02 March, 2023

Question 1

ESL Chapter 5 Figure 5.6 is replicated, the code is shown as below.

```r
# Question 1
# Replicate ESL Chapter 5 Figure 5.6

# Import dataset
bone <- read.table('https://hastie.su.domains/ElemStatLearn/datasets/bone.data',
                   header = TRUE)

# According to ESL Figure 5.6 description, spnbmd is the target variable
# and age is the predictor.

# Plot the age against relative change in spinal BMD, color separated by gender.
plot(x = bone$age, y = bone$spnbmd,
     col = ifelse(bone$gender == 'female','red','blue'),
     pch = 20, xlab = 'Age', ylab = 'Relative Change in Spinal BMD')

# Split male and female.
male_bone <- bone[bone$gender == 'male', ]
female_bone <- bone[bone$gender == 'female', ]

# Spline, using degree of freedom = 12 (given by the textbook)
male_spline <- smooth.spline(x = male_bone$age, y = male_bone$spnbmd, df = 12)
female_spline <- smooth.spline(x = female_bone$age, y = female_bone$spnbmd, df = 12)
```
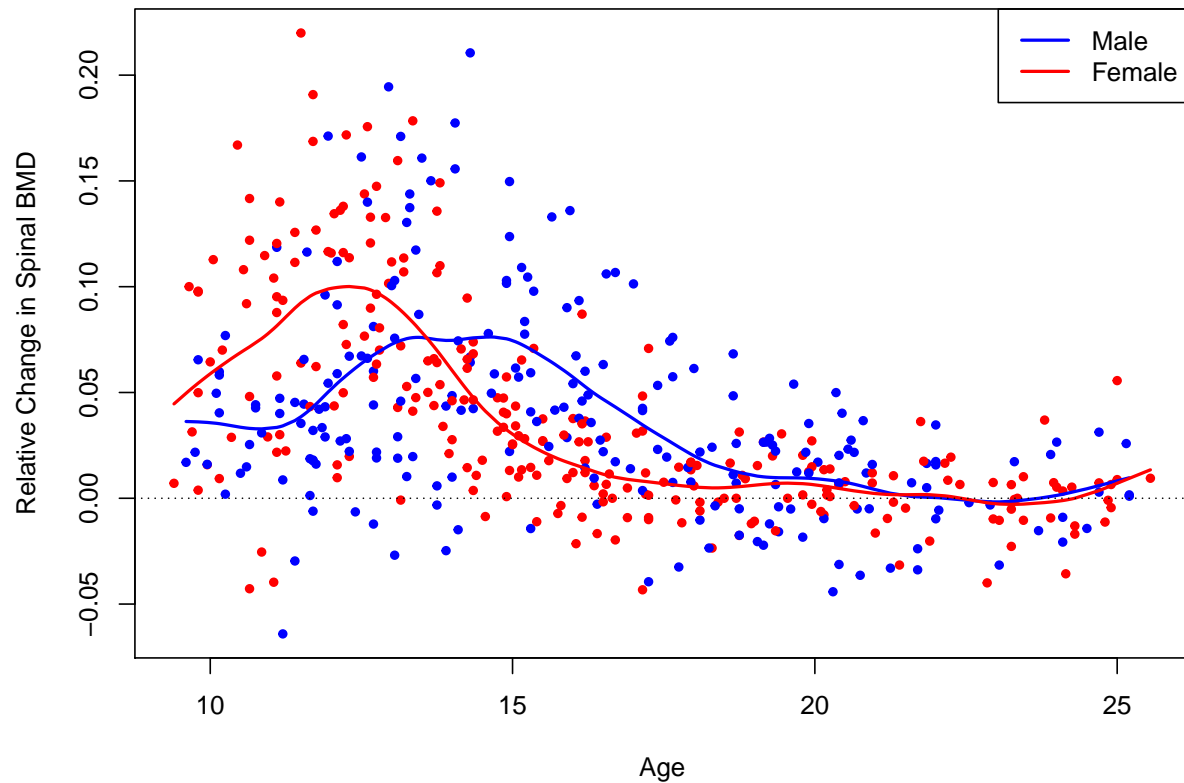
```
# Add splines to the graph with corresponding color for each gender.
lines(male_spline, col = 'blue', lwd = 2)
lines(female_spline, col = 'red', lwd = 2)


# Add a horizontal dash line at y = 0.
abline(h=0, lty=3)


# Add a legend at the top right corner.
legend(x='topright', legend=c('Male', 'Female'),
       col=c('blue', 'red'), lwd=2)
```


Question 2 (South Africa coronary heart disease data)

```
# Question 2
# Import libraries
```

```r
library(splines)
library(ggplot2)


# Import South Africa coronary heart disease data.
url <- "http://www-stat.stanford.edu/~tibs/ElemStatLearn/datasets/SAheart.data"
heart <- read.csv(url, row.names = 1)


# Create a list of 5 knots location for the bases
# Knots that can equally divide the tobacco range are chosen
# There are 107 out of 462 tobacco values are 0, 107/462 = 0.2316
# So the first knot need to be greater than 0.2316 to avoid NA values in glm
knots <- quantile(heart$tobacco, probs = c(0.24, 0.40, 0.55, 0.70, 0.85))


# B-spline base
b_spline <- bs(heart$tobacco, knots = knots)


# Natural spline base
n_spline <- ns(heart$tobacco, knots = knots)


# Truncated polynomial base
# Below is the function that creates truncated polynomial spline base
# it is modified based on Dr. Bolker's code
truncpolyspline <- function(x, knots) {
  trunc_fun <- function(k) (x > k)*(x-k)^3
  S <- sapply(knots, trunc_fun)
  S <- cbind(x, x^2, x^3, S)
  return(S)
}


poly_spline <- truncpolyspline(heart$tobacco, knots) # create basis matrix


# Fit logistic regression
# b-spline
logistic_b <- glm(chd ~ b_spline, data = heart, family = 'binomial')
# natural spline
logistic_n <- glm(chd ~ n_spline, data = heart, family = 'binomial')
```

```r
# truncated polynomial spline
logistic_poly <- glm(chd ~ poly_spline, data = heart, family = 'binomial')


# Predict without using predict() function on log-odds scale
# b-spline
X_b <- model.matrix(logistic_b) # design matrix for b-spline
coef_b <- as.vector(logistic_b$coefficients) # coefficients vector for b-spline
Y_b <- X_b %*% coef_b # predicted value
var_Y_b <- diag(X_b %*% vcov(logistic_b) %*% t(X_b)) # predicted variance
se_Y_b <- as.matrix(sqrt(var_Y_b)) # predicted se
upper_b <- Y_b + se_Y_b # upper bound of the CI
lower_b <- Y_b - se_Y_b # lower bound of the CI


# Create a dataframe for b-spline x, predicted y, upper and lower bound of y.
df_b <- as.data.frame(cbind(heart$tobacco, Y_b, upper_b, lower_b))
colnames(df_b) <- c('tobacco', 'pred', 'upper', 'lower')


# Plot for b-spline
ggplot(df_b, aes(x=tobacco)) +  geom_point(aes(y = pred)) + # scatter plot for Y_b
  geom_line(aes(y = upper), linetype = 'dashed', color = 'red') + # add upper bound
  geom_line(aes(y = lower), linetype = 'dashed', color = 'red') +  # add lower bound
  labs(x = "Tobacco consumption", y = "Fitted value in log-odds scale",
       title = "B-Spline prediction") # add axis labels
```
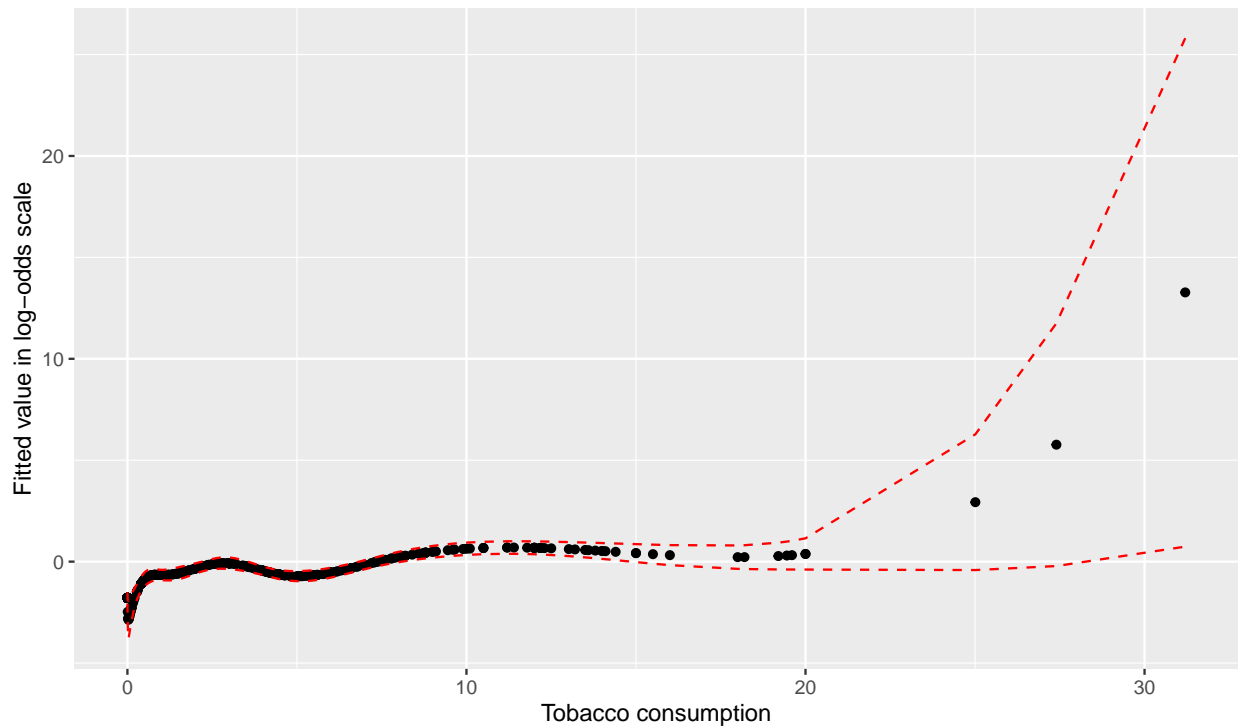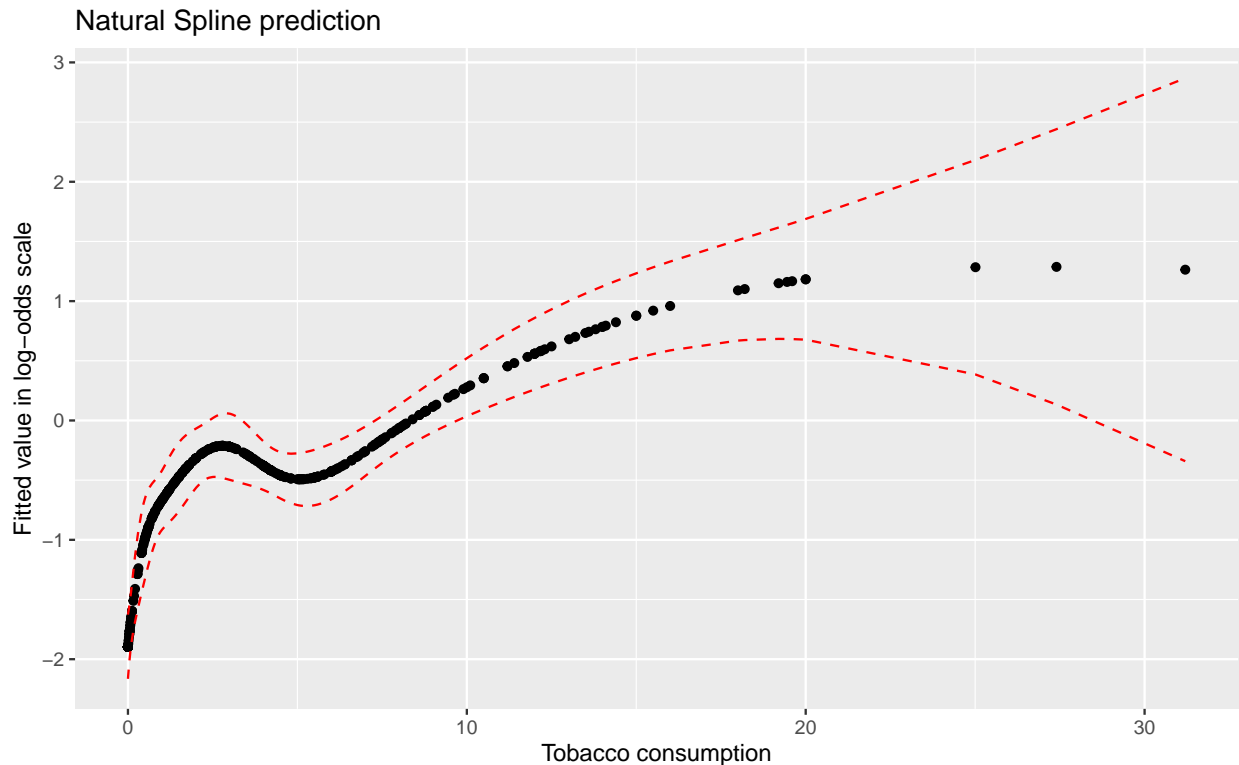
B–Spline prediction


```r
# natural spline
X_n <- model.matrix(logistic_n) # design matrix for b-spline
coef_n <- as.vector(logistic_n$coefficients) # coefficients vector for b-spline
Y_n <- X_n %*% coef_n # predicted value
var_Y_n <- diag(X_n %*% vcov(logistic_n) %*% t(X_n)) # predicted variance
se_Y_n <- as.matrix(sqrt(var_Y_n)) # predicted se
upper_n <- Y_n + se_Y_n # upper bound of the CI
lower_n <- Y_n - se_Y_n # lower bound of the CI


# Create a dataframe for natural spline x, predicted y, upper and lower bound of y.
df_n <- as.data.frame(cbind(heart$tobacco, Y_n, upper_n, lower_n))
colnames(df_n) <- c('tobacco', 'pred', 'upper', 'lower')


# Plot for natural spline
ggplot(df_n, aes(x=tobacco)) +  geom_point(aes(y = pred)) + # scatter plot for Y_b
  geom_line(aes(y = upper), linetype = 'dashed', color = 'red') + # add upper bound
  geom_line(aes(y = lower), linetype = 'dashed', color = 'red') +  # add lower bound
  labs(x = "Tobacco consumption", y = "Fitted value in log-odds scale",
       title = "Natural Spline prediction") # add axis labels
```
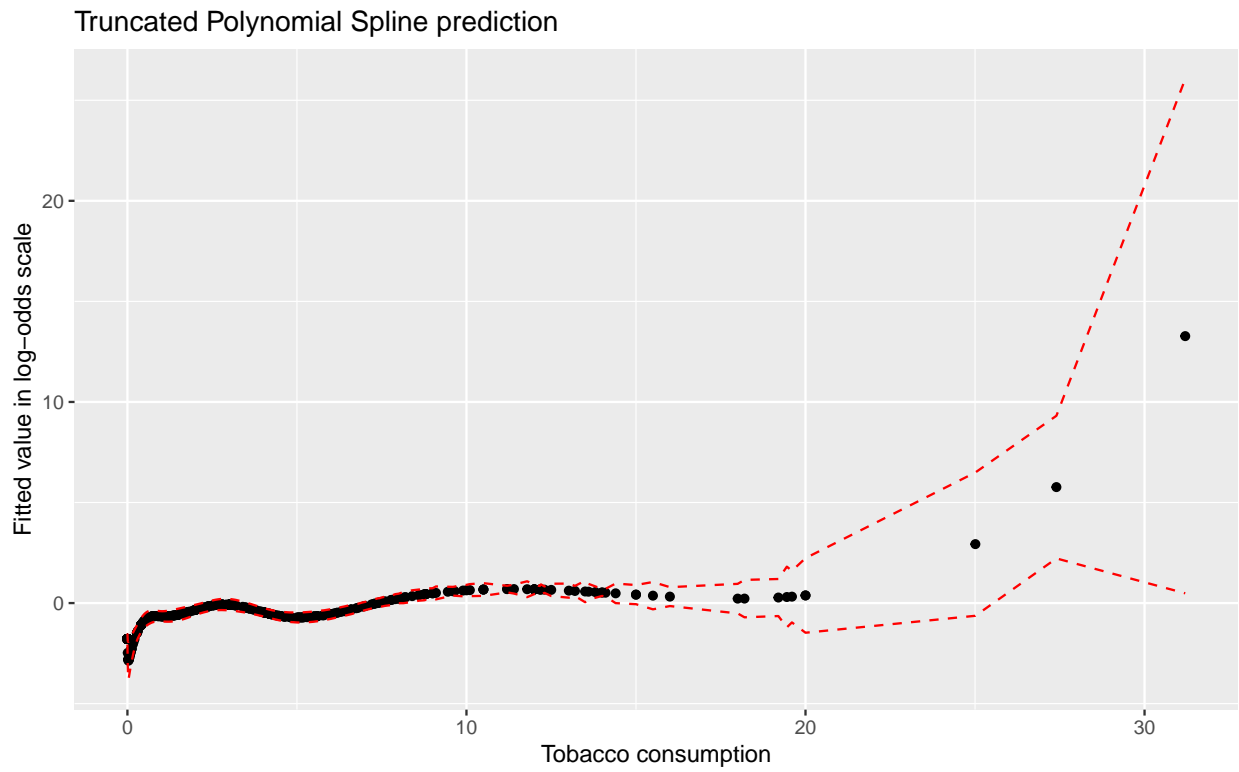
Natural Spline prediction


```r
# truncated polynomial spline
X_poly <- model.matrix(logistic_poly) # design matrix for b-spline
coef_poly <- as.vector(logistic_poly$coefficients) # coefficients vector for b-spline
Y_poly <- X_poly %*% coef_poly # predicted value
var_Y_poly <- diag(X_poly %*% vcov(logistic_poly) %*% t(X_poly)) # predicted variance
se_Y_poly <- as.matrix(sqrt(abs(var_Y_poly))) # predicted se
upper_poly <- Y_poly + se_Y_poly # upper bound of the CI
lower_poly <- Y_poly - se_Y_poly # lower bound of the CI


# Create a dataframe for truncated polynomial spline x, predicted y,
# upper and lower bound of y.
df_poly <- as.data.frame(cbind(heart$tobacco, Y_poly, upper_poly, lower_poly))
colnames(df_poly) <- c('tobacco', 'pred', 'upper', 'lower')


# Plot for truncated polynomial spline
ggplot(df_poly, aes(x=tobacco)) +  geom_point(aes(y = pred)) + # scatter plot for Y_b
  geom_line(aes(y = upper), linetype = 'dashed', color = 'red') + # add upper bound
  geom_line(aes(y = lower), linetype = 'dashed', color = 'red') +  # add lower bound
  labs(x = "Tobacco consumption", y = "Fitted value in log-odds scale",
```

```
            title = "Truncated Polynomial Spline prediction") # add axis labels
```

Truncated Polynomial Spline prediction
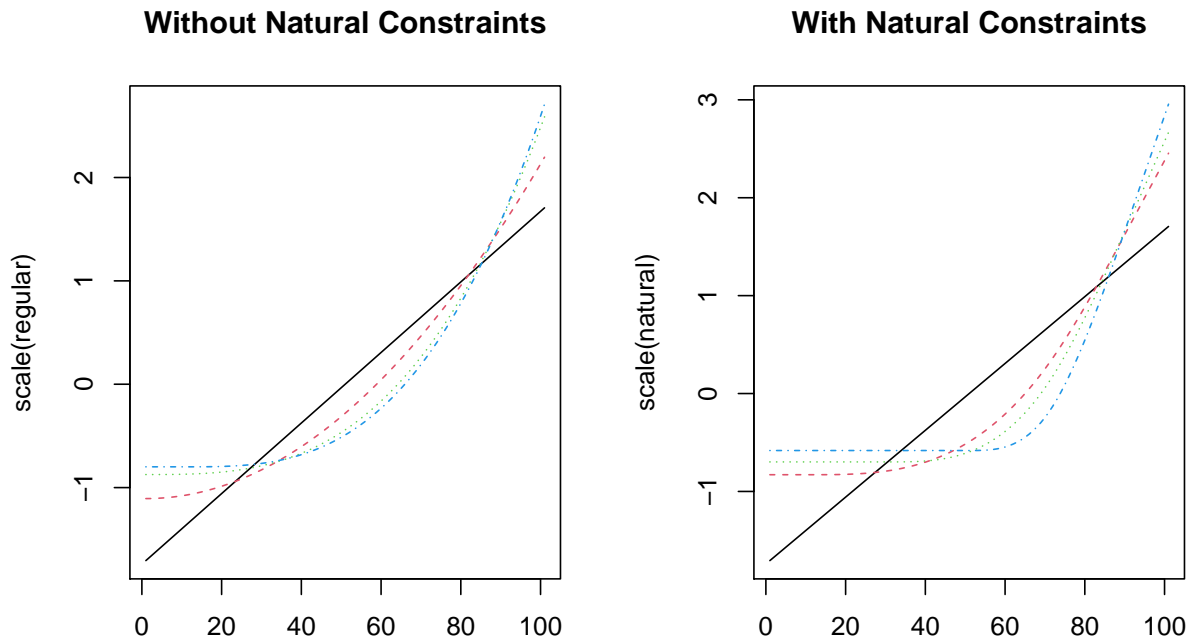

Question 3

```
# Write a function that adds natural spline constraint on truncated polynomial.
truncPoly <- function(x, df, natural = TRUE) {
  # x is the predictor
  # df is degree of freedom
  # natural is a boolean argument determining if natural constraint is needed
  if (natural){
    K <- df # df = K for natural, K is the number of knots
    knots <- quantile(x, seq(0.1, 0.9, length = K)) # obtain K knots
    # d_k(X) is a matrix with n rows and K-1 columns
    d_k <- matrix(NA, nrow = length(x), ncol = K-1)
    for (i in 1:(K-1)){
      numerator <- (x > knots[i])*(x-knots[i])^3 - (x > knots[K])*(x-knots[K])^3
      denominator <- knots[K]-knots[i]
      d_k[,i] <- numerator/denominator # ESL(5.5)
```

```r
  }
  # N_{k+2}(X) is a matrix with n rows and K-2 columns
  N_kplus2 <- matrix(NA, nrow = length(x), ncol = K-2)
  for (i in 1:(K-2)){
    N_kplus2[,i] <- d_k[,i] - d_k[,K-1] # ESL(5.4)
  }
  # Final matrix of basis, N_2(X) = X, N_{k+2}(X) defined as above
  N <- cbind(x, N_kplus2)
  return(N)
  }
  else {
    K <- df - 4 # df = K+4 for regular
    knots <- quantile(x, seq(0.1, 0.9, length = K)) # obtain K knots
    trunc_fun <- function(k) (x > k)*(x-k)^3
    S <- sapply(knots[1:(df-2)], trunc_fun)
    S <- cbind(x, x^2, x^3, S) # regular truncated polynomial spline
    return(S)
  }
}


# Plot an example of regular and natural bases
x <- seq(0, 10, length = 101) # example from lecture
regular <- truncPoly(x, df = 5, natural = FALSE) # regular bases
natural <- truncPoly(x, df = 5, natural = TRUE) # natural bases
# Plots
par(mfrow = c(1, 2))
matplot(scale(regular), type = "l", main = "Without Natural Constraints")
matplot(scale(natural), type = "l", main = "With Natural Constraints")
```

Without Natural Constraints **With Natural Constraints**

Question 4

```r
# Part(a)
# Simulate data from a surface on the unit square with Gaussian noise
my_simulation <- function(n, noise_mean = 0, noise_sd = 1){
  # n is the number of observations required
  # noise_mean is the mean of the noise term, default is 0
  # noise_sd if the sd of the noise term, default is 1

  # draw numbers from unit square x-axis
  x <- runif(n)
  # draw numbers from unit square y-axis
  y <- runif(n)
  # noise term from Gaussian distribution
  noise <- rnorm(n, noise_mean, noise_sd)
  # create a smooth surface using a high-order bivariate polynomial
  z <- 5*x^7*y^6 + 2*x^6*y^5 + x^5 + 7*x^3*y^2 + 2*x^2*y + x*y^2 + y^3 + 3*y^4*x + y^8
  # smooth surface with gaussian noise
```

9

```r
  z_noise <- z + noise
  # return a data frame with three columns: x, y, and z
  data.frame(x = x, y = y, z = z_noise)
}


# Example of the simulation
# Expect a list of 5 numbers that are generated using the polynomial above
# and with noises from a Gaussian distribution with mean 0.5 and sd 2.5.
my_simulation(5, 0.5, 2.5)$z
```

```
## [1]  1.28827918 -3.08361235  0.74278007  0.05808562  3.15579991
```

```r
# Part (b)
# Import libraries
library(mgcv)


# Function below returns the true value of z, used to compare with the prediction
true_z <- function(x, y){
  5*x^7*y^6 + 2*x^6*y^5 + x^5 + 7*x^3*y^2 + 2*x^2*y + x*y^2 + y^3 + 3*y^4*x + y^8
}


# 250 simulations
simulation_num <- 250


# (i) method = "GCV.Cp".
# Create an empty matrices to store the computed value for each simulation
comp_time1 <- matrix(NA, nrow=simulation_num, ncol=1)
bias1 <- matrix(NA, nrow=simulation_num, ncol=1)
variance1 <- matrix(NA, nrow=simulation_num, ncol=1)
mse1 <- matrix(NA, nrow=simulation_num, ncol=1)


for (i in 1:simulation_num) {
  # Simulate 500 random samples for each simulation with standard gaussian noise
  my_data <- my_simulation(500, 0, 1)


  # Fit a GAM model using z ~ te(x,y) formula and method = "GCV.Cp"
```

```r
  start_time <- Sys.time() # time before running model
  model1 <- gam(z ~ te(x,y,bs = "gp"), data = my_data, method = "GCV.Cp")
  end_time <- Sys.time() # time after running model
  comp_time1[i] <- as.numeric(end_time - start_time) # computation time


  # Create test set using runif()
  x_test <- runif(50)
  y_test <- runif(50)
  test_set <- as.data.frame(cbind(x = x_test, y = y_test))


  # Prediction
  pred <- predict(model1, newdata = test_set) # predicted z value
  true <- true_z(x_test, y_test) # true value of z for comparison


  # Compute bias, variance, and MSE of the predictions
  bias1[i] <- mean(pred - true)
  variance1[i] <- mean((pred - mean(pred))^2)
  mse1[i] <- mean((pred - true)^2)
}


mean(comp_time1)
```

```
## [1] 0.1279299
```

```r
mean(bias1)
```

```
## [1] 0.001493343
```

```r
mean(variance1)
```

```
## [1] 8.347659
```

```r
mean(mse1)
```

```
## [1] 0.05777512
```

```r
# (ii) method = "REML".
# Create an empty matrices to store the computed value for each simulation
comp_time2 <- matrix(NA, nrow=simulation_num, ncol=1)
bias2 <- matrix(NA, nrow=simulation_num, ncol=1)
variance2 <- matrix(NA, nrow=simulation_num, ncol=1)
mse2 <- matrix(NA, nrow=simulation_num, ncol=1)

for (i in 1:simulation_num) {
  # Simulate 500 random samples for each simulation with standard gaussian noise
  my_data <- my_simulation(500, 0, 1)

  # Fit a GAM model using z ~ te(x,y) formula and method = "REML"
  start_time <- Sys.time()
  model2 <- gam(z ~ te(x,y,bs = "gp"), data = my_data, method = "REML")
  end_time <- Sys.time()
  comp_time2[i] <- as.numeric(end_time - start_time) # computation time

  # Create test set using runif()
  x_test <- runif(50)
  y_test <- runif(50)
  test_set <- as.data.frame(cbind(x = x_test, y = y_test))

  # Prediction
  pred <- predict(model2, newdata = test_set) # predicted z value
  true <- true_z(x_test, y_test) # true value of z for comparison

  # Compute bias, variance, and MSE of the predictions
  bias2[i] <- mean(pred - true)
  variance2[i] <- mean((pred - mean(pred))^2)
  mse2[i] <- mean((pred - true)^2)
}

mean(comp_time2)
```

```
## [1] 0.1533553
```

12

```
mean(bias2)
```

```
## [1] -0.002745222
```

```
mean(variance2)
```

```
## [1] 8.224685
```

```
mean(mse2)
```

```
## [1] 0.0639727
```

```
# Create a comparison table for two methods
compare <- matrix(c(mean(comp_time1), mean(bias1), mean(variance1), mean(mse1),
                    mean(comp_time2), mean(bias2), mean(variance2), mean(mse2)),
                  ncol = 2, nrow = 4)
colnames(compare) <- c("GCV.Cp", "REML")
rownames(compare) <- c("computation time", "bias", "variance", "mse")
compare
```

```
##                        GCV.Cp         REML
## computation time 0.127929921  0.153355270
## bias             0.001493343 -0.002745222
## variance         8.347658852  8.224684938
## mse              0.057775120  0.063972703
```

```
# Generally, both methods have similar computation time, bias, variance and mse.
# REML has slightly greater values in all outputs.
```

Question 5

ESL 5.4   The natural boundary conditions for natural cubic splines is that "the function is linear beyond the boundary knots". When $X < \xi_1$, $f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$, to make it linear, we need β_2 and β_3 equal to 0. Alternatively, we can prove by taking the second derivative of f(x) and set it to 0. $f''(x) = 2\beta_2 + 6\beta_3 x = 0$, hence $\beta_2 = \beta_3 = 0$.

Similarly, the function f(x) should be linear when $X > \xi_k$ where $f(x) = \beta_0 + \beta_1 x + \sum_{k=1}^{K} \theta_k (X - \xi_k)^3$, we take second derivative and set it to 0. $f''(x) = 6 \sum_{k=1}^{K} \theta_k (X - \xi_k) = 6(\sum_{k=1}^{K} \theta_k X - \sum_{k=1}^{K} \theta_k \xi_k) = 0$, then we have $\sum_{k=1}^{K} \theta_k X - \sum_{k=1}^{K} \theta_k \xi_k = 0$, which implies that $\sum_{k=1}^{K} \theta_k = 0$ and $\sum_{k=1}^{K} \theta_k \xi_k = 0$, as required.

Now we derive (5.4) and (5.5). The function we have is $f(x) = \beta_0 + \beta_1 x + \sum_{k=1}^{K} \theta_k (X - \xi_k)_+^3 = 0$, by observing the function, we get that $N_1(X) = 1, N_2(X) = X$, we now want to prove that $\sum_{k=1}^{K} \theta_k (X - \xi_k)_+^3$ can be written is the form of $N_{k+2}(X) = d_k(X) - d_{k-1}(X)$.

Given that $\sum_{k=1}^{K} \theta_k = 0$ and $\sum_{k=1}^{K} \theta_k \xi_k = 0$, we know that $\sum_{k=1}^{K-2} \theta_k = -\theta_K - \theta_{K-1}$ and $\sum_{k=1}^{K-2} \theta_k \xi_k = -\theta_K \xi_K - \theta_{K-1} \xi_{K-1}$.

$$\sum_{k=1}^{K} \theta_k (X - \xi_k)_+^3 = \sum_{k=1}^{K-2} \theta_k (X - \xi_k)_+^3 + \theta_{K-1}(X - \xi_{K-1})_+^3 + \theta_K (X - \xi_K)_+^3$$

$$
\begin{aligned}
\theta_{K-1}(X - \xi_{K-1})_+^3 &= \theta_{K-1}(X - \xi_{K-1})_+^3 \frac{\xi_{K-1} - \xi_K}{\xi_{K-1} - \xi_K} \\
&= \frac{(X - \xi_{K-1})_+^3}{\xi_{K-1} - \xi_K}(\theta_{K-1}\xi_{K-1} - \theta_{K-1}\xi_K) \\
&= \frac{(X - \xi_{K-1})_+^3}{\xi_{K-1} - \xi_K}(\theta_{K-1}\xi_{K-1} - \theta_{K-1}\xi_K + \theta_K\xi_K - \theta_K\xi_K) \\
&= \frac{(X - \xi_{K-1})_+^3}{\xi_{K-1} - \xi_K}(\theta_{K-1}\xi_{K-1} + \theta_K\xi_K - \theta_{K-1}\xi_K - \theta_K\xi_K) \\
&= \frac{(X - \xi_{K-1})_+^3}{\xi_{K-1} - \xi_K}(-\sum_{k=1}^{K-2}\theta_k\xi_k + \xi_K\sum_{k=1}^{K-1}\theta_k) \\
&= \frac{(X - \xi_{K-1})_+^3}{\xi_{K-1} - \xi_K}\sum_{k=1}^{K-2}\theta_k(\xi_K - \xi_k) \\
&= \sum_{k=1}^{K-2}\theta_k(\xi_K - \xi_k)\frac{(X - \xi_{K-1})_+^3}{\xi_{K-1} - \xi_K}
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
\theta_K(X - \xi_K)_+^3 &= \frac{(X - \xi_K)_+^3}{\xi_{K-1} - \xi_K}\theta_K(\xi_{K-1} - \xi_K) \\
&= \frac{(X - \xi_K)_+^3}{\xi_{K-1} - \xi_K}(\theta_K\xi_{K-1} - \theta_K\xi_K + \theta_{K-1}\xi_{K-1} - \theta_{K-1}\xi_{K-1}) \\
&= \frac{(X - \xi_K)_+^3}{\xi_{K-1} - \xi_K}(-\xi_{K-1}\sum_{k=1}^{K-2}\theta_K + \sum_{k=1}^{K-2}\theta_k\xi_k) \\
&= \sum_{k=1}^{K-2}\theta_k(\xi_k - \xi_{K-1})\frac{(X - \xi_K)_+^3}{\xi_{K-1} - \xi_K}
\end{aligned}
$$

Put them back together and get:

14

$$\sum_{k=1}^{K} \theta_k (X - \xi_k)_+^3 = \sum_{k=1}^{K-2} \theta_k (X - \xi_k)_+^3 + \theta_{K-1} (X - \xi_{K-1})_+^3 + \theta_K (X - \xi_K)_+^3$$

$$= \sum_{k=1}^{K-2} \theta_k (X - \xi_k)_+^3 + \sum_{k=1}^{K-2} \theta_k (\xi_K - \xi_k) \frac{(X - \xi_{K-1})_+^3}{\xi_{K-1} - \xi_K} + \sum_{k=1}^{K-2} \theta_k (\xi_k - \xi_{K-1}) \frac{(X - \xi_K)_+^3}{\xi_{K-1} - \xi_K}$$

$$= \sum_{k=1}^{K-2} \theta_k [(X - \xi_k)_+^3 + (\xi_K - \xi_k) \frac{(X - \xi_{K-1})_+^3}{\xi_{K-1} - \xi_K} + (\xi_k - \xi_{K-1}) \frac{(X - \xi_K)_+^3}{\xi_{K-1} - \xi_K}]$$

$$= \sum_{k=1}^{K-2} \theta_k [(X - \xi_k)_+^3 \frac{\xi_K - \xi_k}{\xi_K - \xi_k} + (\xi_K - \xi_k) \frac{(X - \xi_{K-1})_+^3}{\xi_{K-1} - \xi_K} + (\xi_k - \xi_{K-1}) \frac{(X - \xi_K)_+^3}{\xi_{K-1} - \xi_K} \frac{\xi_K - \xi_k}{\xi_K - \xi_k}]$$

$$= \sum_{k=1}^{K-2} \theta_k (\xi_K - \xi_k) [\frac{(X - \xi_k)_+^3}{\xi_K - \xi_k} + \frac{(X - \xi_{K-1})_+^3}{\xi_{K-1} - \xi_K} + (\xi_k - \xi_{K-1}) \frac{(X - \xi_K)_+^3}{(\xi_{K-1} - \xi_K)(\xi_K - \xi_k)}]$$

$$= \sum_{k=1}^{K-2} \theta_k (\xi_K - \xi_k) [\frac{(X - \xi_k)_+^3}{\xi_K - \xi_k} + \frac{(X - \xi_{K-1})_+^3}{\xi_{K-1} - \xi_K} + (X - \xi_K)_+^3 (\frac{-1}{\xi_{K-1} - \xi_K} - \frac{1}{\xi_K - \xi_k})]$$

$$= \sum_{k=1}^{K-2} \theta_k (\xi_K - \xi_k) [\frac{(X - \xi_k)_+^3 - (X - \xi_K)_+^3}{\xi_K - \xi_k} + \frac{(X - \xi_{K-1})_+^3 - (X - \xi_K)_+^3}{\xi_{K-1} - \xi_K}]$$

$$= \sum_{k=1}^{K-2} \theta_k (\xi_K - \xi_k) [\frac{(X - \xi_k)_+^3 - (X - \xi_K)_+^3}{\xi_K - \xi_k} - \frac{(X - \xi_{K-1})_+^3 - (X - \xi_K)_+^3}{\xi_K - \xi_{K-1}}]$$

$$= \sum_{k=1}^{K-2} \theta_k (\xi_K - \xi_k)(d_k(X) - d_{K-1}(X))$$

$$= \sum_{k=1}^{K-2} \theta_k (\xi_K - \xi_k) N_{k+2}(X)$$

Therefore, to conclude, we get $N_1(X) = 1, N_2(X) = X, N_{k+2}(X) = d_k(X) - d_{K-1}(X)$ as desired in (5.4) and (5.5).

ESL 5.13   From ESL Chapter 5 we learned that smoothing spline is the function f which minimizes the RSS $= \sum_{i=1}^{N}(y_i - f(x_i))^2 + \lambda \int (f''(t))^2 dt$, where λ is the smoothing parameter. If λ is large, then f will be smooth. And if $\lambda \to \infty$, then f will be perfectly smooth like a straight line. Therefore, when we augment our dataset with $(x_0, \hat{f}_\lambda(x_0))$ when λ is very large, then the fitted curve will not change rapidly, the augmented pair has little effect. On the other hand, if λ is small, augmenting the pair $(x_0, \hat{f}_\lambda(x_0))$ will make the smoothing spline more flexible and interpolate the training observations closer.

By the definition of the MSE of n-fold cross validation (leave-one-out cross validation), $MSE = \frac{1}{N} \sum_{i=1}^{N} MSE_i$, where MSE_i is the MSE of each fit, for $i = 1, \ldots, N$. Let $\hat{f}_\lambda^{(-i)}(x_i)$ be the estimate for the ith fit, where (x_i, y_i) is left out. Then $MSE_i = (y_i - \hat{f}_\lambda^{(-i)}(x_i))^2$. Hence by the definition of n-fold cross validation, $MSE_{CV} = \frac{1}{N} \sum_{i=1}^{N}(y_i - \hat{f}_\lambda^{(-i)}(x_i))^2$ (ESL 5.26).

ESL 5.14 states that $\hat{f}_\lambda = S_\lambda y$, then $\hat{f}_\lambda(x_i) = \sum_{j=1}^{n} S_\lambda(i, j) y_j$.

For the estimate at the ith fit, we can also write:

$$\hat{f}_\lambda^{(-i)}(x_i) = \sum_{j=1, j \neq i}^{n} S_\lambda(i,j)y_j + S_\lambda(i,i)y_i$$

$$= \sum_{j=1}^{n} S_\lambda(i,j)y_j - S_\lambda(i,i)y_i + S_\lambda(i,i)y_i$$

$$= \sum_{j=1}^{n} S_\lambda(i,j)y_j - S_\lambda(i,i)y_i + S_\lambda(i,i)\hat{f}_\lambda^{(-i)}(x_i)$$

$$= \hat{f}_\lambda(x_i) - S_\lambda(i,i)y_i + S_\lambda(i,i)\hat{f}_\lambda^{(-i)}(x_i)$$

Therefore,

$$\hat{f}_\lambda^{(-i)}(x_i)(1 - S_\lambda(i,i)) = \hat{f}_\lambda(x_i) - S_\lambda(i,i)y_i$$

$$\hat{f}_\lambda^{(-i)} = \frac{\hat{f}_\lambda(x_i) - S_\lambda(i,i)y_i}{1 - S_\lambda(i,i)}$$

$$y_i - \hat{f}_\lambda^{(-i)} = y_i - \frac{\hat{f}_\lambda(x_i) - S_\lambda(i,i)y_i}{1 - S_\lambda(i,i)}$$

$$y_i - \hat{f}_\lambda^{(-i)} = \frac{y_i - S_\lambda(i,i)y_i - \hat{f}_\lambda(x_i) + S_\lambda(i,i)y_i}{1 - S_\lambda(i,i)}$$

$$y_i - \hat{f}_\lambda^{(-i)} = \frac{y_i - \hat{f}_\lambda(x_i)}{1 - S_\lambda(i,i)}$$

Substitute this result into (5.26) and get $MSE_{CV}(\hat{f}_\lambda) = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{f}_\lambda^{(-i)}(x_i))^2 = \frac{1}{N}\sum_{i=1}^{N}[\frac{y_i - \hat{f}_\lambda(x_i)}{1 - S_\lambda(i,i)}]^2$.

Reference

- Hastie, T., Tibshirani, R., Friedman, J. (2009). The Elements of Statistical Learning: Data Mining, Inference, and Prediction, Second Edition. Springer.
- James, G., Witten, D., Hastie, T., Tibshirani, R. (2021). An Introduction to Statistical Learning with Applications in R, Second Edition. Springer.
- Bolker, B. (2023). Splines and basis expansion (week 3). GitHub. https://github.com/bbolker/stat790/blob/main/notes/splines.qmd
- ahstat. (2015). Why are the basis functions for natural cubic splines expressed as they are? (ESL). Cross Validated. https://stats.stackexchange.com/questions/172217/why-are-the-basis-functions-for-natural-cubic-splines-expressed-as-they-are-es
- COOLSerdash. (2021). Splines: relationship of knots, degree and degrees of freedom. Cross Validated. https://stats.stackexchange.com/questions/517375/splines-relationship-of-knots-degree-and-degrees-of-freedom