STATS 790 Assignment 3

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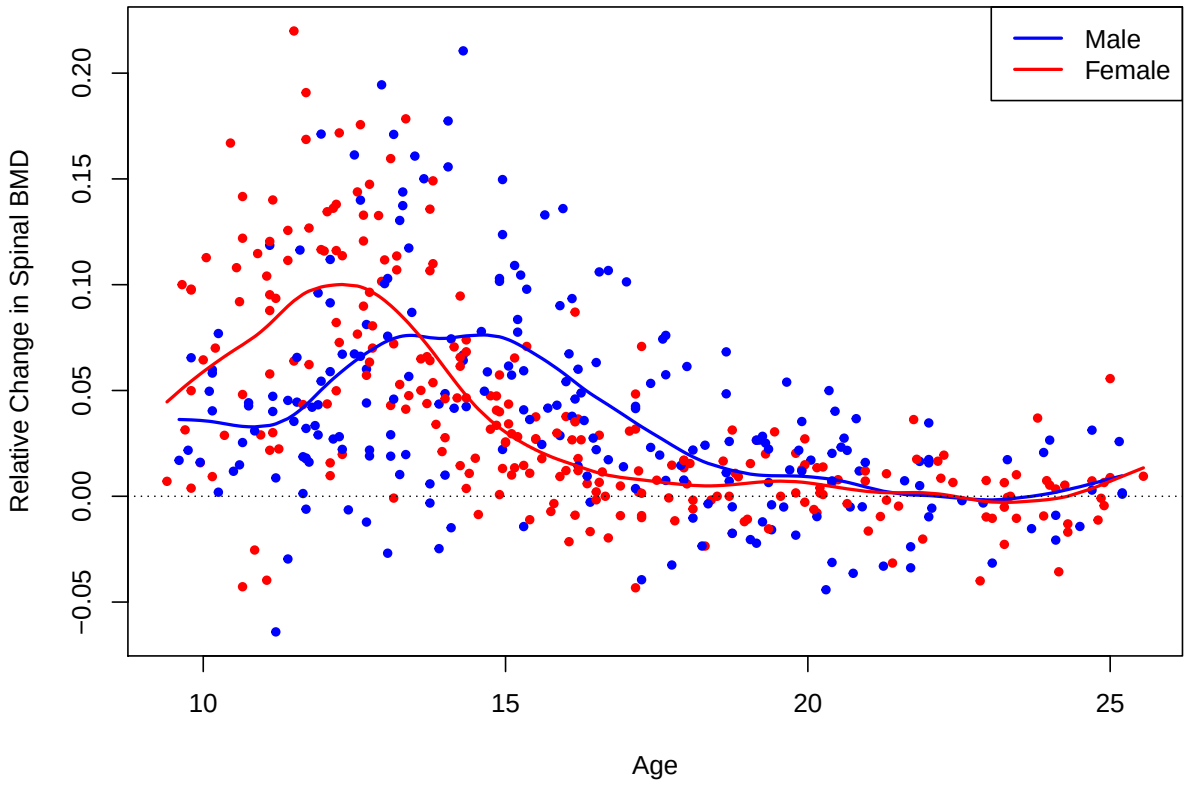
Question 1

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

```
# 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)

# 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, 0.32, 0.48, 0.64, 0.8))

# 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')
# truncated polynomial spline
```

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


summary(logistic_b)
```

```
##
## Call:
## glm(formula = chd ~ b_spline, family = "binomial", data = heart)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -1.4715  -0.9664  -0.5571   1.1216   2.2391
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)  -1.7847     0.2754  -6.480  9.2e-11 ***
## b_spline1    -1.1409     1.3165  -0.867  0.38614
## b_spline2     0.4664     0.9044   0.516  0.60610
## b_spline3     0.9577     0.7068   1.355  0.17541
## b_spline4     1.9666     0.6685   2.942  0.00326 **
## b_spline5     0.8839     0.4749   1.861  0.06271 .
## b_spline6     4.1247     1.4180   2.909  0.00363 **
## b_spline7    -0.6081     3.5395  -0.172  0.86359
## b_spline8     7.8131     6.3520   1.230  0.21869
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 596.11  on 461  degrees of freedom
## Residual deviance: 536.41  on 453  degrees of freedom
## AIC: 554.41
##
## Number of Fisher Scoring iterations: 6
```

```
summary(logistic_n)
```

```
##
## Call:
## glm(formula = chd ~ n_spline, family = "binomial", data = heart)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -1.6808  -0.9949  -0.5417   1.1911   1.9959
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)  -1.8451     0.2721  -6.781 1.19e-11 ***
## n_spline1     1.2904     0.6570   1.964 0.049536 *
## n_spline2     1.7463     0.6477   2.696 0.007020 **
## n_spline3     1.2176     0.4130   2.948 0.003193 **
## n_spline4     2.7821     0.8006   3.475 0.000511 ***
## n_spline5     3.2544     1.1073   2.939 0.003292 **
## n_spline6     3.4619     1.7030   2.033 0.042078 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 596.11  on 461  degrees of freedom
## Residual deviance: 538.76  on 455  degrees of freedom
## AIC: 552.76
##
## Number of Fisher Scoring iterations: 4
```

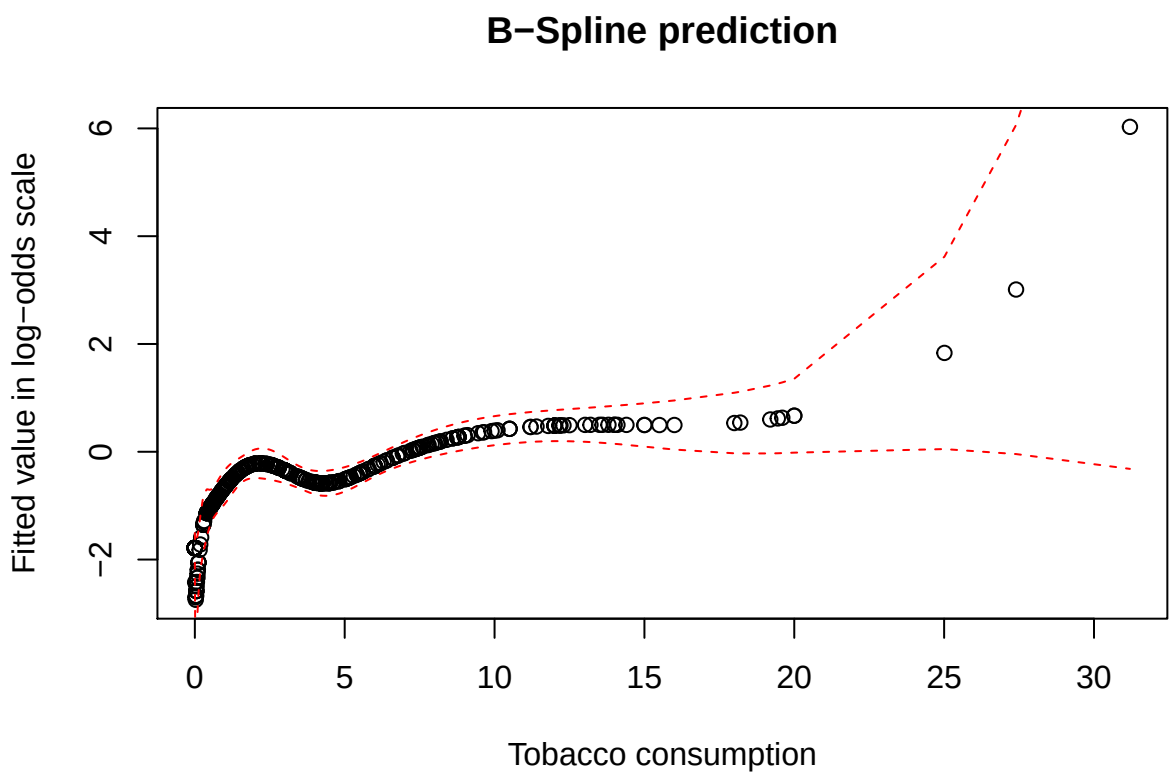
```
summary(logistic_poly)
```

```
##
## Call:
## glm(formula = chd ~ poly_spline, family = "binomial", data = heart)
##
```

```
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -1.4715  -0.9664  -0.5571   1.1216   2.2392
##
## Coefficients:
##                  Estimate Std. Error z value Pr(>|z|)
## (Intercept)    -1.785e+00  2.754e-01  -6.480  9.2e-11 ***
## poly_splinex   -8.557e+01  9.873e+01  -0.867    0.386
## poly_spline     2.385e+03  2.712e+03   0.880    0.379
## poly_spline    -2.003e+04  2.278e+04  -0.879    0.379
## poly_spline24%  2.004e+04  2.280e+04   0.879    0.379
## poly_spline32% -1.358e+01  2.074e+01  -0.655    0.513
## poly_spline48%  1.729e-01  6.612e-01   0.262    0.794
## poly_spline64% -1.211e-01  9.278e-02  -1.305    0.192
## poly_spline80%  3.744e-02  2.453e-02   1.526    0.127
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 596.11  on 461  degrees of freedom
## Residual deviance: 536.41  on 453  degrees of freedom
## AIC: 554.41
##
## Number of Fisher Scoring iterations: 6
```

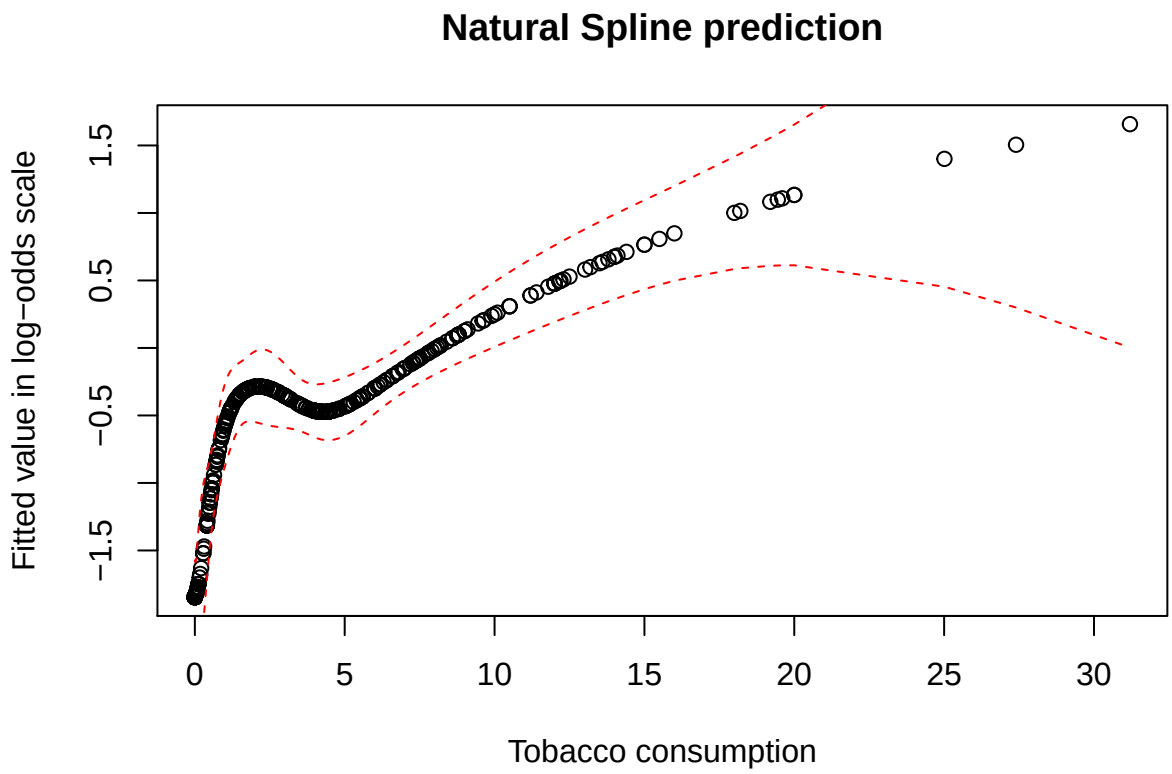
```r
# Predict without using predict() function on log-odds scale
# b-spline
X_b <- model.matrix(logistic_b) # design matrix for b-spline
coef_b <- as.vector(logistic_b$coefficients) # coefficients vector for b-spline
Y_b <- X_b %*% coef_b # predicted value
var_Y_b <- diag(X_b %*% vcov(logistic_b) %*% 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
# Plot the predicted values
```

```r
plot(heart$tobacco, Y_b,
     xlab = 'Tobacco consumption',
     ylab = 'Fitted value in log-odds scale',
     main = 'B-Spline prediction')
# Upper bound
lines(sort(heart$tobacco), upper_b[order(heart$tobacco)], col = "red", lty = 2)
# Lower bound
lines(sort(heart$tobacco), lower_b[order(heart$tobacco)], col = "red", lty = 2)
```



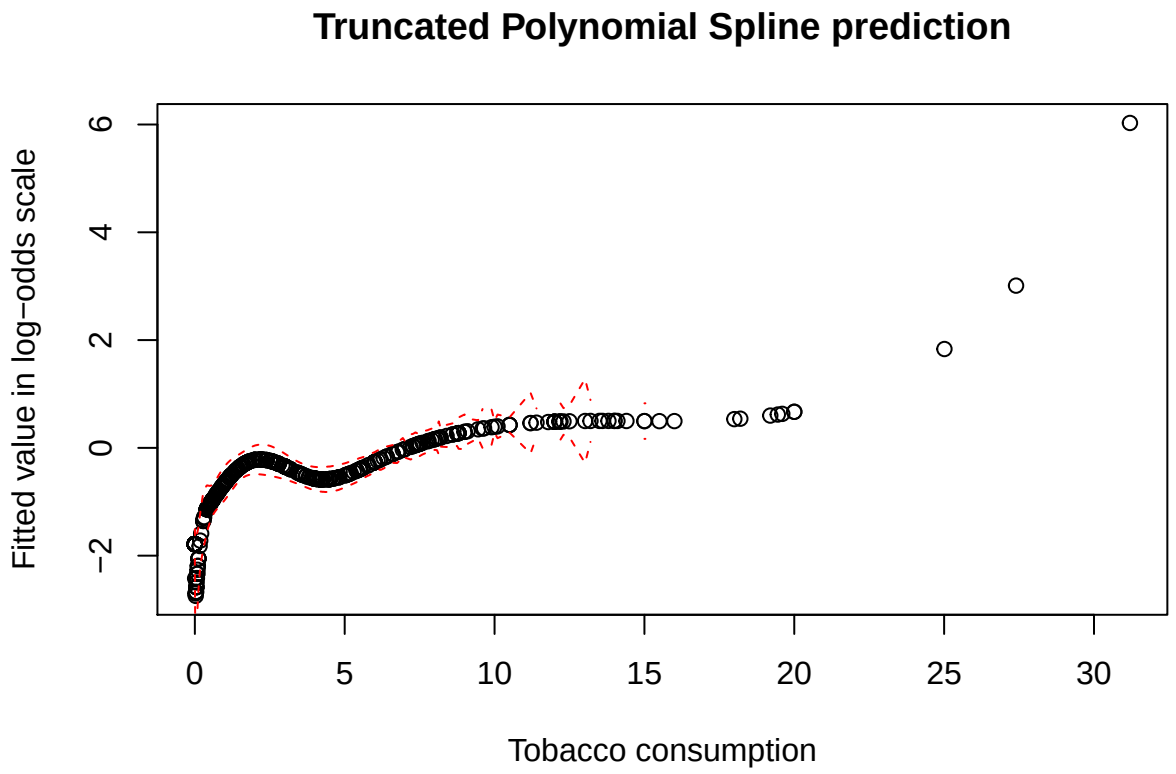

```r
# natural spline
X_n <- model.matrix(logistic_n) # design matrix for b-spline
coef_n <- as.vector(logistic_n$coefficients) # coefficients vector for b-spline
Y_n <- X_n %*% coef_n # predicted value
var_Y_n <- diag(X_n %*% vcov(logistic_n) %*% t(X_n)) # predicted variance
se_Y_n <- as.matrix(sqrt(var_Y_n)) # 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
```

```r
# Plot the predicted values
plot(heart$tobacco, Y_n,
     xlab = 'Tobacco consumption',
     ylab = 'Fitted value in log-odds scale',
     main = 'Natural Spline prediction')
# Upper bound
lines(sort(heart$tobacco), upper_n[order(heart$tobacco)], col = "red", lty = 2)
# Lower bound
lines(sort(heart$tobacco), lower_n[order(heart$tobacco)], col = "red", lty = 2)
```




```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(var_Y_poly)) # predicted se
upper_poly <- Y_poly + se_Y_poly # upper bound of the CI
```

```r
lower_poly <- Y_poly - se_Y_poly # lower bound of the CI
# Plot the predicted values
plot(heart$tobacco, Y_poly,
     xlab = 'Tobacco consumption',
     ylab = 'Fitted value in log-odds scale',
     main = 'Truncated Polynomial Spline prediction')
# Upper bound
lines(sort(heart$tobacco), upper_poly[order(heart$tobacco)], col = "red", lty = 2)
# Lower bound
lines(sort(heart$tobacco), lower_poly[order(heart$tobacco)], col = "red", lty = 2)
```



Question 3 (..)

Question 4 (..)

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:

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

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