STATS 790
Assignment #3

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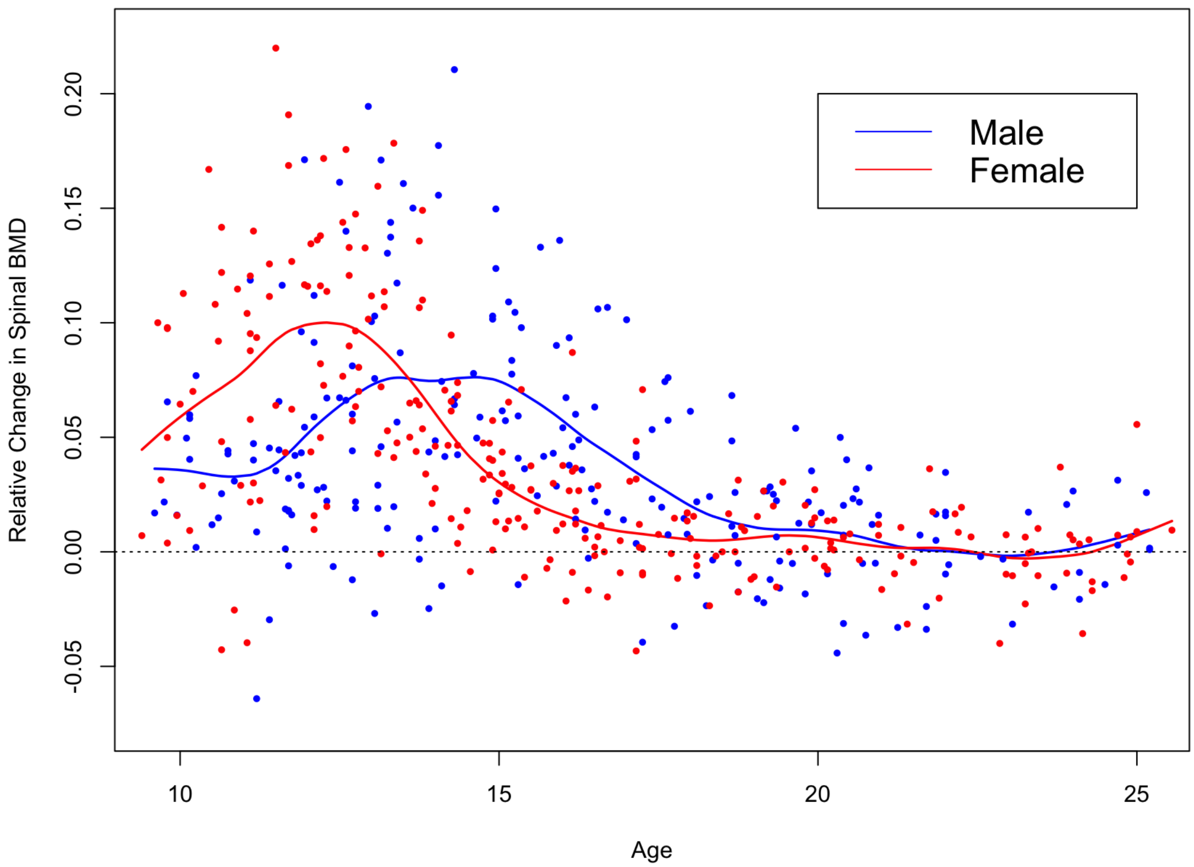
Contents

Question #1

Here we replicate Figure 5.6 from ESL.

```r
#download dataset
url <- "https://hastie.su.domains/ElemStatLearn/datasets/bone.data"
dd_bmd <- read.delim(url)

#create male and female datasets
males <- dd_bmd %>% filter(gender == "male") %>% select(age, spnbmd)
females <- dd_bmd %>% filter(gender == "female") %>% select(age, spnbmd)

#smooth splines
males_spline <- smooth.spline(x = males$age, y = males$spnbmd, df = 12)
females_spline <- smooth.spline(x = females$age, y = females$spnbmd, df = 12)

#code to generate figure
plot(males_spline,ylim=c(-0.075,0.225),col="blue",type="l",
     lwd=1.75,xlab="",ylab="")
lines(females_spline,col="red",lwd=1.75)
points(x=males$age,y=males$spnbmd,col="blue",pch=20,lwd=0.001)
points(x=females$age,y=females$spnbmd,col="red",pch=20,lwd=0.001)
abline(h=0,lty=3)
title(xlab="Age",ylab="Relative Change in Spinal BMD")
legend(x=c(20,25),y=c(0.15,0.20),legend=c("Male","Female"),
       col=c("blue","red"),lty=1,cex=1.5)
```


Male
Female
Relative Change in Spinal BMD
-0.05
0.00
0.05
0.10
0.15
0.20
10
15
20
25
Age

Question #2

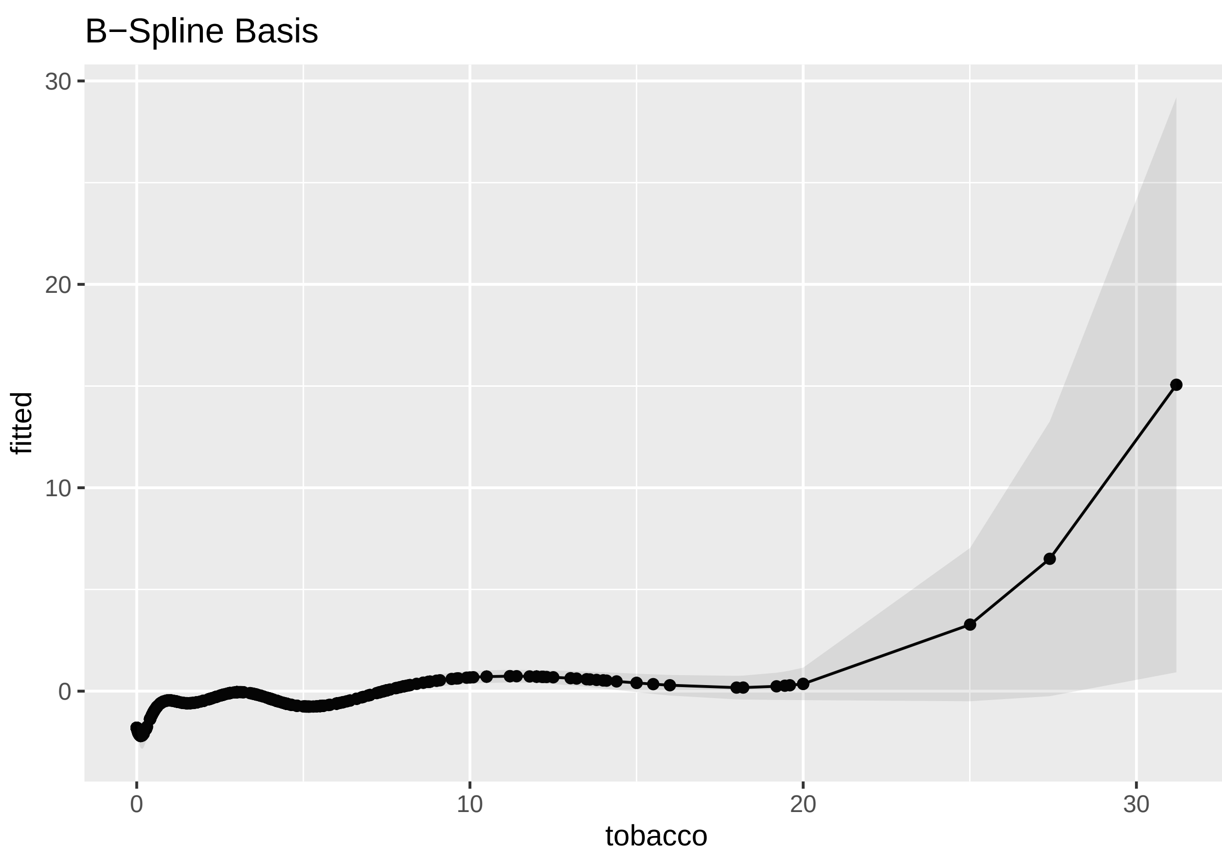
Here we compute a logistic regression model using the b-spline, natural spline and truncated power basis functions.

Custom knots were defined prior to fitting each model as the splines package defaults would produce NA values in the covariance matrix and the truncated power basis function did as well unless the lowest knot was moved to 0.30. Thus, all knots have been placed at the same quantiles so the basis can be compared easily.

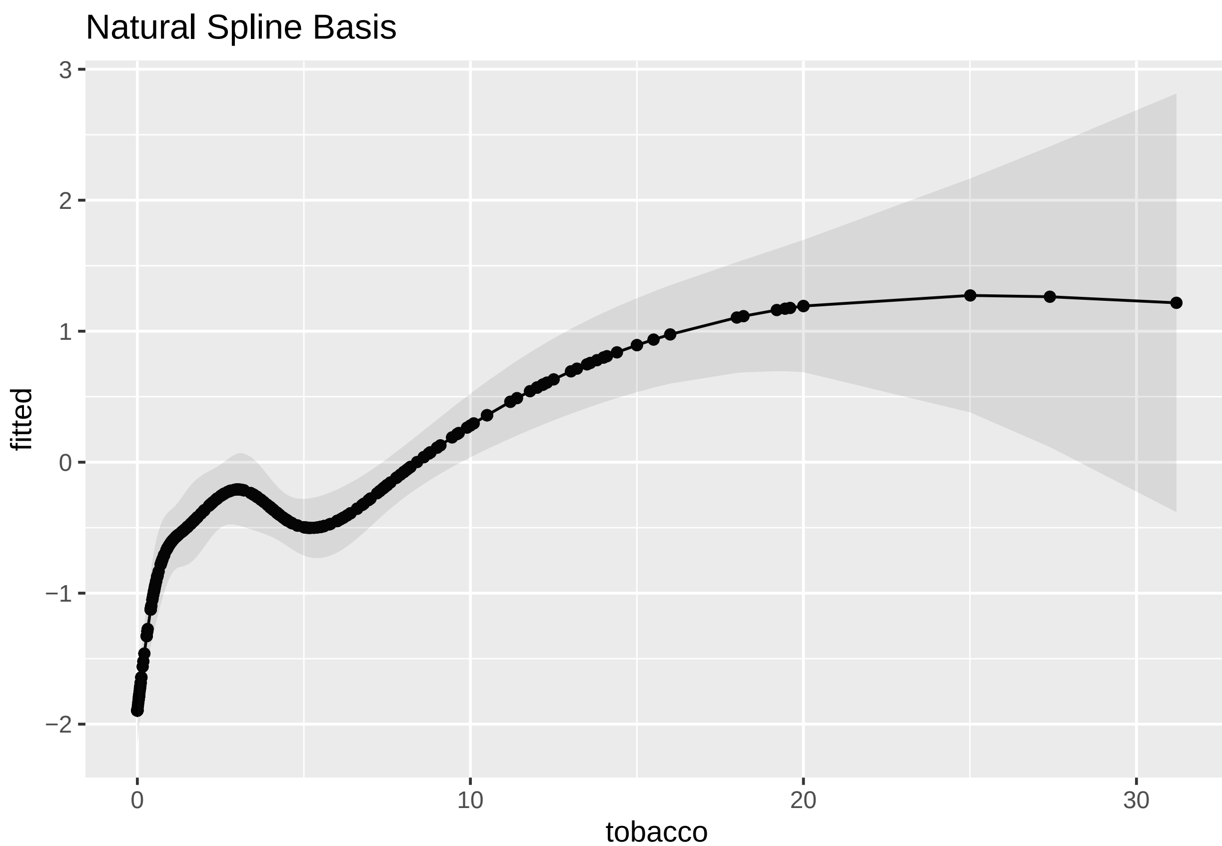
```
#download dataset (borrowed from class notes)
url <- "http://www-stat.stanford.edu/~tibs/ElemStatLearn/datasets/SAheart.data"
fn <- "SAheart.txt"
if (!file.exists(fn)) download.file(url, destfile = fn)
raw_dd <- read.csv(fn, row.names = 1)
dd <- raw_dd %>% select(tobacco, chd)

#b-spline basis
b_spline_fit <- gam(chd ~ bs(x = tobacco, knots = quantile(tobacco, seq(0.30,0.85,length=5))), family = binomial, data = dd)
b_spline_X <- model.matrix(b_spline_fit)
vcov_b <- vcov(b_spline_fit)

#natural spline basis
natural_spline_fit <- gam(chd ~ ns(x = tobacco, knots = quantile(tobacco, seq(0.30,0.85,length=5))), family = binomial, data = dd)
natural_spline_X <- model.matrix(natural_spline_fit)
vcov_natural <- vcov(natural_spline_fit)

#truncated power basis
q2 <- function(x, nknots) {
  knots <- quantile(x, seq(0.30, 0.85, length = nknots))
  trunc_fun <- function(k) (x>=k)*(x-k)^3
  s <- sapply(knots, trunc_fun)
  s <- cbind(x, x^2, x^3, s)
  return(s)
}

truncated_fit <- gam(chd ~ q2(x = tobacco, nknots = 5), family = binomial, data = dd)
truncated_X <- model.matrix(truncated_fit)
vcov_truncated <- vcov(truncated_fit)
```

Plots of the model predictions +/- one standard error on log-odds scale.

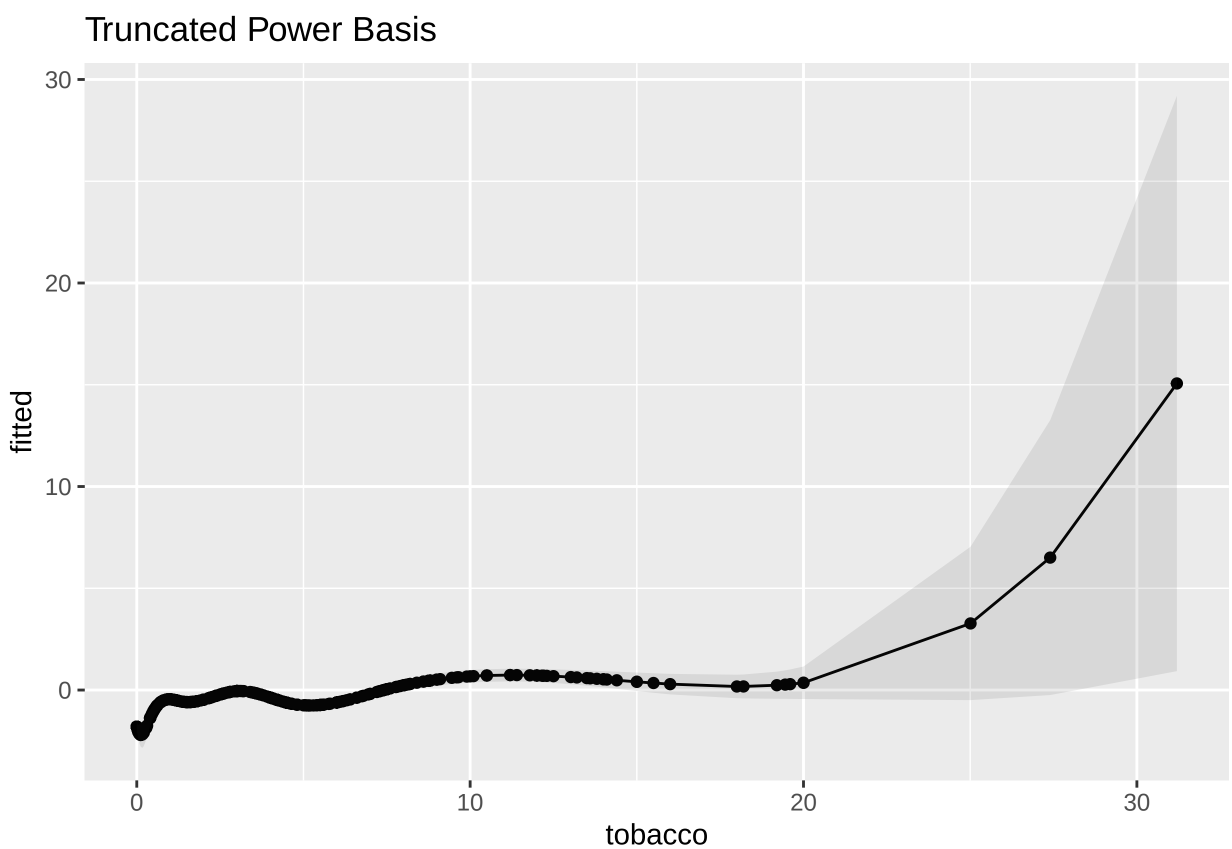
```
#b-spline basis
b_spline_se <- b_spline_X %*% vcov_b %*% t(b_spline_X)
b_spline_se <- sqrt(diag(b_spline_se))
b_spline_plot <- data.frame(tobacco = dd$tobacco,
                            fitted = b_spline_X %*% coef(b_spline_fit),
                            se = b_spline_se)

ggplot(b_spline_plot, aes(x = tobacco, y = fitted)) +
  geom_line() +
  geom_point() +
  geom_ribbon(aes(ymin = fitted - se, ymax = fitted + se), alpha = 0.1) +
  labs(title = "B-Spline Basis")
```



```r
#natural spline basis
natural_spline_se <- natural_spline_X %*% vcov_natural %*% t(natural_spline_X)
natural_spline_se <- sqrt(diag(natural_spline_se))
natural_spline_plot <- data.frame(tobacco = dd$tobacco,
                                  fitted = natural_spline_X %*% coef(natural_spline_fit),
                                  se = natural_spline_se)

ggplot(natural_spline_plot, aes(x = tobacco, y = fitted)) +
  geom_line() +
  geom_point() +
  geom_ribbon(aes(ymin = fitted - se, ymax = fitted + se), alpha = 0.1) +
  labs(title = "Natural Spline Basis")
```



```
#truncated power basis
truncated_se <- truncated_X %*% vcov_truncated %*% t(truncated_X)
truncated_se <- sqrt(diag(truncated_se))
truncated_plot <- data.frame(tobacco = dd$tobacco,
                                  fitted = truncated_X %*% coef(truncated_fit),
                                  se = truncated_se)

ggplot(truncated_plot, aes(x = tobacco, y = fitted)) +
  geom_line() +
  geom_point() +
  geom_ribbon(aes(ymin = fitted - se, ymax = fitted + se), alpha = 0.1) +
  labs(title = "Truncated Power Basis")
```



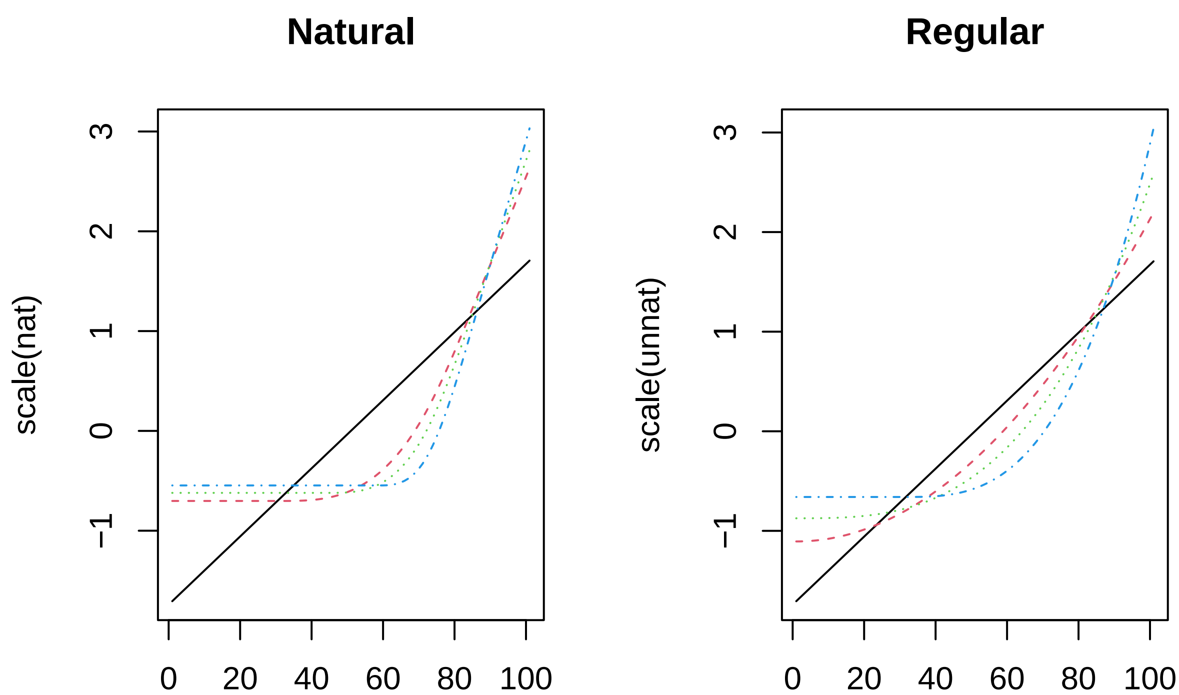
Question #3

Below we create a function that implements the truncated power basis and natural spline basis.

```r
truncpolyspline <- function(x, df, natural = c(TRUE, FALSE)) {
  if (!require("Matrix")) stop("need Matrix package")

  #truncated power basis
  if(!natural) {
    knots <- quantile(x, seq(0.30, 0.85, length = df - 4))

    trunc_fun <- function(k) (x>=k)*(x-k)^3

    s <- sapply(knots, trunc_fun)
    s <- cbind(x, x^2, x^3, s)
    return(s)
  }

  #natural spline basis
  if(natural) {
    knots <- quantile(x, seq(0.30, 0.85, length = df))

    trunc_fun <- function(k, K, d_K_1) {
      ((x>=k)*(x-k)^3 - (x>=K)*(x-K)^3)/(K-k) - d_K_1
    }

    K <- as.numeric(knots[length(knots)])
    K_1 <- as.numeric(knots[length(knots)-1])
    d_K_1 <- ((x>=K_1)*(x-K_1)^3 - (x>=K)*(x-K)^3)/(K-K_1)

    s <- sapply(knots[1:df],trunc_fun,K=K, d_K_1=d_K_1)
    s <- cbind(x, s)
    return(s)
  }
}
```

Below we plot the basis functions for $df = 5$ as in the notes.

```
xvec <- seq(0, 10, length = 101)
nat <- truncpolyspline(xvec, df = 5, natural = TRUE)
unnat <- truncpolyspline(xvec, df = 5, natural = FALSE)
par(mfrow = c(1, 2))
matplot(scale(nat), type = "l", main = "Natural")
matplot(scale(unnat), type = "l", main = "Regular")
```



Question #4

a) Here we simulate data from the two-dimensional surface $f(x, y) = \exp((x - \frac{1}{2})^2 + (y - \frac{1}{2})^2)$ with points drawn uniform at random on the x and y axis.

```
sim_values <- function(c1 = 1/2, c2 = 1/2) {
  x <- runif(1)
  y <- runif(1)
  f <- exp((x-c1)^2+(y-c2)^2) + rnorm(1)
  return(list(x,y,f))
}

df <- data.frame(x=rep(0, 250), y=rep(0, 250), z=rep(0, 250))
for (i in 1:250) df[i,] <- df[i,] + sim_values()
```

b) Use mgcv::gam() to fit two-dimensional splines to your simulated data, using z ~ te(gp, x, y). Over an ensemble of 250 simulations, compute the average computation time, bias, variance, and mean-squared error of your predictions for (i) method = "GCV.Cp" (generalized cross-validation) and (ii) method = "REML" (restricted maximum likelihood).

```
mgcv::gam(z ~ te(x,y), data = df, method = "GCV.Cp")
```

```
##
## Family: gaussian
## Link function: identity
##
## Formula:
## z ~ te(x, y)
##
## Estimated degrees of freedom:
## 19  total = 19.98
##
## GCV score: 1.071899
```

```
mgcv::gam(z ~ te(x,y), data = df, method = "REML")
```

```
##
## Family: gaussian
## Link function: identity
##
## Formula:
## z ~ te(x, y)
##
## Estimated degrees of freedom:
## 4.4  total = 5.4
##
## REML score: 363.2344
```

Question #5 (ESL 5.4)

Consider the truncated power series representation for cubic splines with K interior knots:

$$f(X) = \sum_{j=0}^{3} \beta_j X^j + \sum_{k=1}^{K} \theta_k (X - \xi_k)_+^3$$

The natural boundary conditions say that outside the boundary knots, the function must be linear. For $X < \xi_1$, we have $\sum_{k=1}^{K} \theta_k (X-\xi_k)_+^3 = 0$ and $f(X) = \sum_{j=0}^{3} \beta_j X^j = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3$. For this function to be linear when $X < \xi_1$, we have $\beta_2 = \beta_3 = 0$. Similarly for $X \geq \xi_k$, we have $f(X) = \sum_{j=0}^{3} \beta_j X^j + \sum_{k=1}^{K} \theta_k (X-\xi_k)_+^3$. Expanding the second term we have $(X-\xi_k)_+^3 = X^3 - 3\xi_k X^2 + 3\xi_k^2 X - \xi_k^3$.

We can re-write $f(X)$ in the following way:

$$\begin{aligned}
f(X) &= \sum_{j=0}^{3} \beta_j X^j + \sum_{k=1}^{K} \theta_k (X - \xi_k)_+^3 && (1)\\
&= \sum_{j=0}^{3} \beta_j X^j + \sum_{k=1}^{K} \theta_k [X^3 - 3\xi_k X^2 + 3\xi_k^2 X - \xi_k^3] && (2)\\
&= \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \sum_{k=1}^{K} \theta_k X^3 - 3\sum_{k=1}^{K} \theta_k \xi_k X^2 + 3\sum_{k=1}^{K} \theta_k \xi_k^2 X - \sum_{k=1}^{K} \theta_k \xi_k^3 && (3)\\
&= \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \sum_{k=1}^{K} \theta_k X^3 - 3\sum_{k=1}^{K} \theta_k \xi_k X^2 + 3\sum_{k=1}^{K} \theta_k \xi_k^2 X - \sum_{k=1}^{K} \theta_k \xi_k^3 && (4)\\
&= \beta_0 - \sum_{k=1}^{K} \theta_k \xi_k^3 + X(\beta_1 + 3\sum_{k=1}^{K} \theta_k \xi_k^2) + X^2(\beta_2 - 3\sum_{k=1}^{K} \theta_k \xi_k) + X^3(\beta_3 + \sum_{k=1}^{K} \theta_k) && (5)
\end{aligned}$$

For this function to be linear, we require $\beta_2 - 3\sum_{k=1}^{K} \theta_k \xi_k = 0$ and $\beta_3 + \sum_{k=1}^{K} \theta_k = 0$. Further, we have $\beta_2 = \beta_3 = 0$, which implies $\sum_{k=1}^{K} \theta_k \xi_k = 0$ and $\sum_{k=1}^{K} \theta_k = 0$ as required.

The natural cubic spline basis is of the form $N_1(X) = 1$, $N_2(X) = X$ and $N_{k+2}(X) = d_k(X) - d_{K-1}(X)$ where $d_k(X) = \frac{(X-\xi_k)_+^3 - (X-\xi_K)_+^3}{\xi_K - \xi_k}$. To derive this basis from the truncated power series representation, we show that $f(X)$ can be written as a linear combination of the $N_k(X)$ basis functions such that $f(X) = \sum_{k=1}^{K} \alpha_k N_k(X)$.

For $X < \xi_1$, we have $N_{k+2}(X) = d_k(X) - d_{K-1}(X) = 0$ for all $k > 2$ which means

$$f(X) = \sum_{k=1}^{K} \alpha_k N_k(X) = \alpha_1 N_1(X) + \alpha_2 N_2(X) = \alpha_1 + \alpha_2 X$$

Thus, we have $\alpha_1 = \beta_0$ and $\alpha_2 = \beta_1$.

For $X \geq \xi_K$ and $K - 2 \geq k$, we have the following:

$$\begin{aligned}
N_{k+2}(X) &= d_k(X) - d_{K-1}(X) && (6)\\
&= \tfrac{(X-\xi_k)_+^3-(X-\xi_K)_+^3}{\xi_K-\xi_k} - \tfrac{(X-\xi_{K-1})_+^3-(X-\xi_K)_+^3}{\xi_K-\xi_{K-1}} && (7)\\
&= \tfrac{X^3-3\xi_k X^2+3\xi_k^2 X-\xi_k^3-X^3+3\xi_K X^2-3\xi_K^2 X+\xi_K^3}{\xi_K-\xi_k} - \tfrac{X^3-3\xi_{K-1}X^2+3\xi_{K-1}^2 X-\xi_{K-1}^3-X^3+3\xi_K X^2-3\xi_K^2 X+\xi_K^3}{\xi_K-\xi_{K-1}} && (8)\\
&= \tfrac{(-3\xi_k+3\xi_K)X^2+(3\xi_k^2-3\xi_K^2)X+(\xi_K^3-\xi_k^3)}{\xi_K-\xi_k} - \tfrac{(-3\xi_{K-1}+3\xi_K)X^2+(3\xi_{K-1}^2-3\xi_K^2)X+(\xi_K^3-\xi_{K-1}^3)}{\xi_K-\xi_{K-1}} && (9)\\
&= \tfrac{3(\xi_K-\xi_k)X^2+3(\xi_k^2-\xi_K^2)X+(\xi_K^3-\xi_k^3)}{\xi_K-\xi_k} - \tfrac{3(\xi_K-\xi_{K-1})X^2+3(\xi_{K-1}^2-\xi_K^2)X+(\xi_K^3-\xi_{K-1}^3)}{\xi_K-\xi_{K-1}} && (10)\\
&= 3X^2 - 3X^2 + \tfrac{3(\xi_k^2-\xi_K^2)X+(\xi_K^3-\xi_k^3)}{\xi_K-\xi_k} - \tfrac{3(\xi_{K-1}^2-\xi_K^2)X+(\xi_K^3-\xi_{K-1}^3)}{\xi_K-\xi_{K-1}} && (11)\\
&= \tfrac{3(\xi_k+\xi_K)(\xi_k-\xi_K)X+(\xi_K-\xi_k)(\xi_K^2+2\xi_K\xi_k+\xi_k^2)}{\xi_K-\xi_k} - \tfrac{3(\xi_{K-1}+\xi_K)(\xi_{K-1}-\xi_K)X+(\xi_K-\xi_{K-1})(\xi_K^2+2\xi_K\xi_{K-1}+\xi_{K-1}^2)}{\xi_K-\xi_{K-1}} && (12)\\
&= \tfrac{-3(\xi_k+\xi_K)(\xi_K-\xi_k)X}{\xi_K-\xi_k} + \tfrac{(\xi_K-\xi_k)(\xi_K^2+2\xi_K\xi_k+\xi_k^2)}{\xi_K-\xi_k} + \tfrac{3(\xi_{K-1}+\xi_K)(\xi_K-\xi_{K-1})X}{\xi_K-\xi_{K-1}} - \tfrac{(\xi_K-\xi_{K-1})(\xi_K^2+2\xi_K\xi_{K-1}+\xi_{K-1}^2)}{\xi_K-\xi_{K-1}} && (13)\\
&= -3(\xi_k+\xi_K)X + (\xi_K^2+2\xi_K\xi_k+\xi_k^2) + 3(\xi_{K-1}+\xi_K)X - (\xi_K^2+2\xi_K\xi_{K-1}+\xi_{K-1}^2) && (14)\\
&= (2\xi_K\xi_k+\xi_k^2-2\xi_K\xi_{K-1}-\xi_{K-1}^2) + 3((\xi_{K-1}+\xi_K)-(\xi_k+\xi_K))X && (15)\\
&= b + mX && (16)
\end{aligned}$$

This shows that $f(X)$ is linear past the last boundary knot as required.

Before showing the recursion relation holds for the basis, we need two identities. The first identity is from the first section of the proof:

$$\sum_{k=1}^{K} \theta_k = 0 \tag{17}$$

$$\implies \sum_{k=1}^{K-1} \theta_k = -\theta_K \tag{18}$$

$$\implies \sum_{k=1}^{K-2} \theta_k = -\theta_K - \theta_{K-1} \tag{19}$$

The second identity follows in the same way:

$$\sum_{k=1}^{K} \xi_k \theta_k = 0 \tag{20}$$

$$\implies \sum_{k=1}^{K-2} \xi_k \theta_k = -\xi_K \theta_K - \xi_{K-1}\theta_{K-1} \tag{21}$$

We know from the basis that for the $N_{K+2}(X)$ coefficients, the remaining term should be $\sum_{k=1}^{K} \theta_k (X - \xi_k)_+^3$. For this to happen, we need to multiply the coefficients by a factor of $(\xi_K - \xi_k)$. To see this, we now derive the last part of the basis as follows:

$$(\xi_K - \xi_k) \sum_{k=1}^{K-2} \theta_k N_{K+2}(X) = \sum_{k=1}^{K-2} \theta_k (\xi_K - \xi_k)[\frac{(X-\xi_k)_+^3 - (X-\xi_K)_+^3}{\xi_K - \xi_k} - \frac{(X-\xi_{K-1})_+^3 - (X-\xi_K)_+^3}{\xi_K - \xi_{K-1}}] \tag{22}$$

$$= \sum_{k=1}^{K-2} \theta_k (X-\xi_k)_+^3 - \sum_{k=1}^{K-2} \theta_k (X-\xi_K)_+^3 - \frac{(X-\xi_{K-1})_+^3 - (X-\xi_K)_+^3}{\xi_K - \xi_{K-1}} \sum_{k=1}^{K-2} \theta_k (\xi_K - \xi_k) \tag{23}$$

Using the derived identities from above we get:

$$= \sum_{k=1}^{K-2} \theta_k (X-\xi_k)_+^3 - \sum_{k=1}^{K-2} \theta_k (X-\xi_K)_+^3 - \frac{(X-\xi_{K-1})_+^3 - (X-\xi_K)_+^3}{\xi_K - \xi_{K-1}} (\xi_K \sum_{k=1}^{K-2} \theta_k - \sum_{k=1}^{K-2} \theta_k \xi_k) \tag{24}$$

$$= \sum_{k=1}^{K-2} \theta_k (X-\xi_k)_+^3 - \sum_{k=1}^{K-2} \theta_k (X-\xi_K)_+^3 - \frac{(X-\xi_{K-1})_+^3 - (X-\xi_K)_+^3}{\xi_K - \xi_{K-1}} (-\theta_K \xi_K - \theta_{K-1} \xi_K + \theta_K \xi_K + \theta_{K-1} \xi_{K-1}) \tag{25}$$

$$= \sum_{k=1}^{K-2} \theta_k (X-\xi_k)_+^3 - \sum_{k=1}^{K-2} \theta_k (X-\xi_K)_+^3 - \frac{(X-\xi_{K-1})_+^3 - (X-\xi_K)_+^3}{\xi_K - \xi_{K-1}} (-\theta_{K-1} \xi_K + \theta_{K-1} \xi_{K-1}) \tag{26}$$

$$= \sum_{k=1}^{K-2} \theta_k (X-\xi_k)_+^3 - \sum_{k=1}^{K-2} \theta_k (X-\xi_K)_+^3 + \theta_{K-1} \frac{(X-\xi_{K-1})_+^3 - (X-\xi_K)_+^3}{\xi_K - \xi_{K-1}} (\xi_K - \xi_{K-1}) \tag{27}$$

$$= \sum_{k=1}^{K-2} \theta_k (X-\xi_k)_+^3 - (X-\xi_K)_+^3 \sum_{k=1}^{K-2} \theta_k + \theta_{K-1} ((X-\xi_{K-1})_+^3 - (X-\xi_K)_+^3) \tag{28}$$

$$= \sum_{k=1}^{K-2} \theta_k (X-\xi_k)_+^3 - (X-\xi_K)_+^3 (-\theta_K - \theta_{K-1}) + \theta_{K-1} ((X-\xi_{K-1})_+^3 - (X-\xi_K)_+^3) \tag{29}$$

$$= \sum_{k=1}^{K-2} \theta_k (X-\xi_k)_+^3 + \theta_K (X-\xi_K)_+^3 + \theta_{K-1} (X-\xi_K)_+^3 + \theta_{K-1} (X-\xi_{K-1})_+^3 - \theta_{K-1} (X-\xi_K)_+^3 \tag{30}$$

$$= \sum_{k=1}^{K-2} \theta_k (X-\xi_k)_+^3 + \theta_K (X-\xi_K)_+^3 + \theta_{K-1} (X-\xi_{K-1})_+^3 \tag{31}$$

$$= \sum_{k=1}^{K} \theta_k (X-\xi_k)_+^3 \tag{32}$$

Thus, $\alpha_k = (\xi_K - \xi_k)\theta_k$ and we have shown the two basis representations are equivalent.

Question #6 (ESL 5.13)

Suppose we fit the smoothing spline $\hat{f}_\lambda = S_\lambda y$ where $S_\lambda = N(N^TN + \lambda\Omega_N)^{-1}N^T$. We will use the notation $\hat{f}^{(-i)}(x)$ to denote the prediction made at x_i using a smoothing spline fitted to data that excludes the i^{th} observation. When performing LOOCV, we remove each point and re-fit the model. In vector notation, we can write this out as $y' = y + (\hat{f}_\lambda^{(-i)}(x_i) - y_i)e_i$, where y is the original vector of responses. The vector e_i is the standard basis vector in $\mathbb{R}^N$, and in this representation we replace the i^{th} observation of y with the predicted value $\hat{f}_\lambda^{(-i)}(x_i)$. The fitted values for the response vector y' are:

$$\begin{aligned}
\hat{f}_\lambda^{(-i)} &= S_\lambda y' && (33)\\
&= S_\lambda(y + (\hat{f}_\lambda^{(-i)}(x_i) - y_i)e_i) && (34)\\
&= S_\lambda y + S_\lambda(\hat{f}_\lambda^{(-i)}(x_i) - y_i)e_i && (35)\\
&= \hat{f}_\lambda + S_\lambda(\hat{f}_\lambda^{(-i)}(x_i) - y_i)e_i && (36)
\end{aligned}$$

The term $S_\lambda y$ is equal to fitting the spline using all of the data, which is just $\hat{f}_\lambda$ from above. To get the coordinate for x_i, we can take the dot product with e_i^T as follows:

$$\begin{aligned}
e_i^T\hat{f}_\lambda^{(-i)} &= e_i^T\hat{f}_\lambda + e_i^TS_\lambda(\hat{f}^{(-i)}(x_i) - y_i)e_i && (37)\\
\hat{f}_\lambda^{(-i)}(x_i) &= \hat{f}_\lambda(x_i) + (\hat{f}^{(-i)}(x_i) - y_i)e_i^TS_\lambda e_i && (38)\\
\hat{f}_\lambda^{(-i)}(x_i) &= \hat{f}_\lambda(x_i) + (\hat{f}^{(-i)}(x_i) - y_i)S_\lambda(i,i) && (39)
\end{aligned}$$

We have $e_i^T\hat{f}_\lambda^{(-i)} = \hat{f}_\lambda^{(-i)}(x_i)$ since we are picking out the i^{th} coordinate of the fitted values for y'. Further, $e_i^T\hat{f}_\lambda = \hat{f}_\lambda(x_i)$, which is the predicted value for x_i from the full model. Note that the term $(\hat{f}^{(-i)}(x_i) - y_i)$ is a scalar and the term $S_\lambda(i,i) = e_i^TS_\lambda e_i$ denotes the i^{th} row and column of the smoothing matrix.

To get the form of equation (5.26), we multiply both sides by -1 and add y_i to both sides:

$$y_i - \hat{f}_\lambda^{(-i)}(x_i) = y_i - \hat{f}_\lambda(x_i) - (\hat{f}^{(-i)}(x_i) - y_i)S_\lambda(i,i) \tag{40}$$

$$y_i - \hat{f}_\lambda^{(-i)}(x_i) + (\hat{f}^{(-i)}(x_i) - y_i)S_\lambda(i,i) = y_i - \hat{f}_\lambda(x_i) \tag{41}$$

$$y_i - \hat{f}_\lambda^{(-i)}(x_i) + \hat{f}^{(-i)}(x_i)S_\lambda(i,i) - y_iS_\lambda(i,i) = y_i - \hat{f}_\lambda(x_i) \tag{42}$$

$$y_i(1 - S_\lambda(i,i)) + \hat{f}_\lambda^{(-i)}(x_i)(S_\lambda(i,i) - 1) = y_i - \hat{f}_\lambda(x_i) \tag{43}$$

$$(1 - S_\lambda(i,i))(y_i - \hat{f}_\lambda^{(-i)}(x_i)) = y_i - \hat{f}_\lambda(x_i) \tag{44}$$

$$y_i - \hat{f}_\lambda^{(-i)}(x_i) = \frac{y_i - \hat{f}_\lambda(x_i)}{1 - S_\lambda(i,i)} \tag{45}$$

Thus, we have the N-fold cross validation formula as follows:

$$CV(\hat{f}_\lambda) = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{f}_\lambda^{(-i)}(x_i))^2 \tag{46}$$

$$= \frac{1}{N}\sum_{i=1}^{N}(\frac{y_i - \hat{f}_\lambda(x_i)}{1 - S_\lambda(i,i)})^2 \tag{47}$$