4.5 Splines Regression

Splines are piecewise polynomials thar are constructed so that thay can be both sensitive and smooth, but also capture local features of the data.

A **Cubic Spline** is a curve constructed from sections of cubic polynomials, joined together so that the curve is *continuous up to second derivative*. The points at which the sections join are called the **knots** of the spline. For a conventional spline, the knots occur wherever there is a datum, but for the regression splines the locations of the knots must be chosen. Typically, the knots would either be *evenly spaced* through the range of observed x values, or placed at the *quantiles* of the distribution of unique x values. Each section of cubic has different coefficients, but at the knots *it will match its neighboring sections in value and first two derivatives*.

Cubic Splines (Mathematical) Definition

A function g defined on $[a, b]$ is a **cubic spline** with respect to **knots** $\{\xi_i\}_{i=1}^m$ (specifically $a < \xi_1 < \xi_2 < \ldots < \xi_m < b$) if:

- g is a cubic polynomial in each of the $m + 1$ intervals, i.e.

$$g(x) = d_i x^3 + c_i x^2 + b_i x + a_i, \quad x \in [\xi_i, \xi_{i+1}]$$

  where $i = 0, \ldots, m$, $\xi_0 = a$ and $\xi_{m+1} = b$.

- g is continuous up to the *2nd* derivative. Since g is continuous up to the *2nd* derivative *for any point inside an interval*, it suffices to check the following conditions:

$$g^{(0,1,2)}(\xi_i^+) = g^{(0,1,2)}(\xi_i^-), \quad i = 1, \ldots, m$$

  This expression indicates that the function and the first and second order derivatives are continuous at the knots.

How many free parameters do we need to represent a cubic spline?

(+) 4 parameters (d_i, c_i, b_i, a_i) *for each of the* $(m+1)$ *intervals*.

(-) 3 constraints *at each of the* m *knots* (continuity constraints).

The total number of free parameters (similar to the number of degrees of freedom) is:

$$4(m+1) - 3m = m + 4$$

A property of the cubic splines

Suppose the knots $\{\xi_i\}_{i=1}^m$ are given.

- If $g_1(x)$ and $g_2(x)$ are cubic splines, the linear combination

  $$a_1 g_1(x) + a_2 g_2(x)$$

  is also a cubic spline, where a_1 and a_2 are known constants.

That is, for a set of given knots, the corresponding *cubic splines form a linear space (of functions) with dim* $(m+4)$.

4.5.1 Examples of Cubic Splines Basis

1. A set of basis functions for cubic splines (w.r.t knots $\{\xi_i\}_{i=1}^m$) is given by:

   $$\begin{aligned} h_0(x) &= 1 \\ h_1(x) &= x \\ h_2(x) &= x^2 \\ h_3(x) &= x^3; \\ h_{i+3}(x) &= (x - \xi_i)_+^3, \quad i = 1, 2, \ldots, m \end{aligned}$$

   That is, any cubic spline can be uniquely expressed as:

   $$\beta_0 + \sum_{j=1}^{m+3} \beta_j h_j(x)$$

2. Given knot locations, there are many alternative, but equivalent ways of writing down a basis for cubic splines. For example, *another* basis for cubic splines can be written as:

$$\begin{aligned} h_0(x) &= 1 \\ h_1(x) &= x \\ h_{i+1}(x) &= R(x, \xi_i^*),\ \ i = 1, \ldots, q-1 \end{aligned}$$

where

$$\begin{aligned} R(x,z) = &\left[(z-1/2)^2 - 1/12\right]\left[(x-1/2)^2 - 1/12\right]/4 \\ &- \left[(|x-z|-1/2)^4 - 1/2(|x-z|-1/2)^2 + 7/240\right]/24 \end{aligned}$$

An Example of a Cubic Splines Basis

We first define the function $R(x,z)$ as above in `R` :

```
R_xz <- function(x,z){
  ((z-0.5)^2-1/12)*((x-0.5)^2-1/12)/4-((abs(x-z)-0.5)^4-(abs(x-z)-0.5)^2/2+7/240)
}
```

We then need to define the knots

```
new.knots= c(1/6, 3/6, 5/6)
```

In regression examples the x variable will be the predictor (there is no need to generate any x values). Here, we need a “generic” x for illustration purposes.

```
x=seq(0, 1, by=0.01)
```

Finally, we defined the splines functions, based on the definition given above:

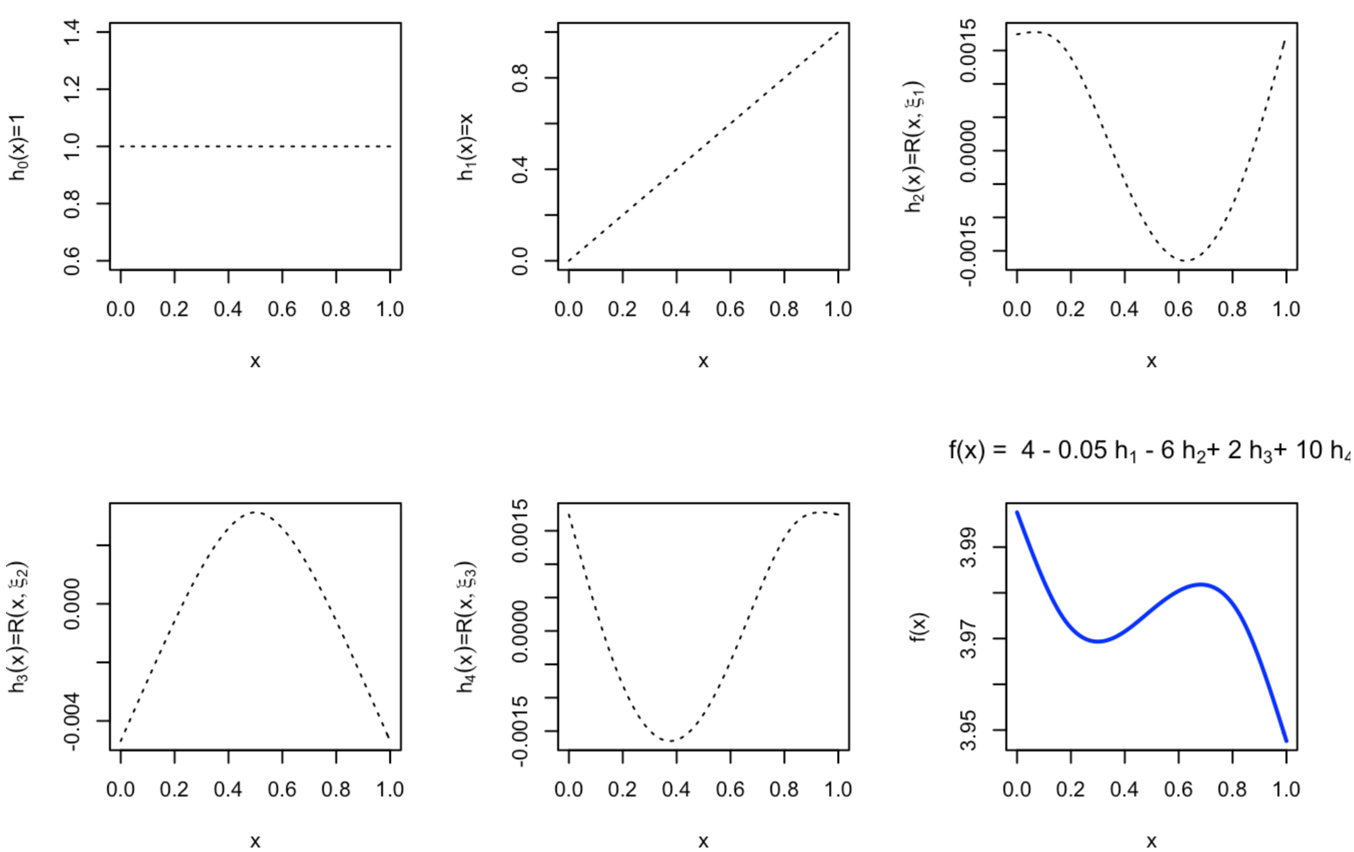
```
spline1 = rep(1, length(x)) # First basis function
spline2 = x # Second basis function
spline3 = R_xz(x,new.knots[1]) # Third basis function
spline4 = R_xz(x,new.knots[2]) # Fourth basis function
spline5 = R_xz(x,new.knots[3]) # Fifth basis function
```

If we want to represent a function using the basis above, we have:

```
fun1s = 4*spline1 - 0.05*spline2 - 6*spline3 +2*spline4 +10*spline5
```

For illustration purposes, we plot the basis functions defined above as well as the function f:

```
par(mfrow = c(2,3))
plot(x, spline1, type='l', lty=3, ylab=expression("h"[0]*"(x)=1"))
plot(x, spline2, type='l',lty=3, ylab=expression("h"[1]*"(x)=x"))
plot(x, spline3, type='l',lty=3, ylab=expression(paste(h[2](x))*"="*paste(R(x,xi[
plot(x, spline4, type='l',lty=3, ylab=expression(paste(h[3](x))*"="*paste(R(x,xi[
plot(x, spline5, type='l',lty=3, ylab=expression(paste(h[4](x))*"="*paste(R(x,xi[
plot(x, fun1s, type='l', ylab="f(x)", main=expression("f(x) =  4 - 0.05 h"[1]*" -
```



4.5.2 B-Splines Basis Functions in `R`

In this class, one of the cubic splines basis that we are to use is called **B-Splines**.

Cubic B Splines Definition

The cubic B Splines basis is defined on an interval $[a, b]$ by the following requirements on the interior basis functions with knotpoints at $\{\xi_i\}_{i=1}^m$:

1. A given basis function is nonzero on an interval defined by four successive knots and zero elsewhere.
2. the basis function is a cubic polynomial for each subinterval between successive knots.
3. The basis function is continuous and is also continuous in its first and second derivatives at each knotpoint.
4. The basis function integrates to 1 over its support.
5. The boundary function definitions are adjusted to account for continuity in derivatives at the boundaries of the interval.

These are part of the `splines` library and the function to generate then is called `bs`. The arguments of the `bs` function are:

$$bs(x, df, knots, degree, intercept, Boundary.knots)$$

The `R` documentation can be found here.

Arguments in the `bs` function:

- `x` is the predictor, i.e. the variable to which we want to apply the splines function.
- `df` are the degrees of freedom for the splines functions.
- `knots` are the *internal* breakpoints/knots that define the spline, i.e. location where the knots should be placed.

- `degree` is the degree of the piecewise polynomial. The default is `degree=3` for cubic splines.
- `intercept` is whether we want to add an intercept in the splines basis or not. *This is not the intercept in the regression we perform*. The default is `intercept=FALSE` .
- `Boundary.knots` are the boundary points at which we "anchor" the B-splines basis. The default values are obtained from the range of non-NA values of `x` , i.e. `Boundary.knots=FALSE` .

So, *in our examples*, we will need to feed the appropriate predictor `x` and then the desired `knots` **or** degrees of freedom, `df` , *not both*. The rest we leave them at their default values.

The **output** of the `bs()` function is a *matrix* of dimension `c(length(x), df)` , if `df` was supplied or of dimension `df = length(knots) + degree (+1 if intercept=TRUE)` if `knots` were supplied.

Knots or Degrees of Freedom in `bs()`

As we mentioned, we need to supply the degrees of freedom or the location of the knots in the `bs()` function, and of course there is an equivalence between the two. Some details to keep in mind on how you can correctly specify these arguments:

- If you know where the knots should be placed, then you need to define a vector of the **locations** of the knots and input that in the `knots` argument in the `bs()` function. For example,

Defining `knots` location in `bs()`

```
library(splines)
x=seq(0, 1, by=0.01) # generic `x` for illustration purposes
new.knots= c(1/6, 3/6, 5/6)  # define three knots at locations 1/6, 3/6, 5/6.
Bsplines.basis1 = bs(x, knots=new.knots)
head(Bsplines.basis1)
```

```
##              1         2         3 4 5 6
## [1,] 0.000000 0.0000000 0.0000000 0 0 0
## [2,] 0.165912 0.0034896 0.0000144 0 0 0
## [3,] 0.304896 0.0135168 0.0001152 0 0 0
## [4,] 0.418824 0.0294192 0.0003888 0 0 0
## [5,] 0.509568 0.0505344 0.0009216 0 0 0
## [6,] 0.579000 0.0762000 0.0018000 0 0 0
```

In this case, `R` calculates the degrees of freedom using the following formula:

$$\mathrm{df} = \mathrm{length(knots)} + \mathrm{degree}$$

or **if** **`intercept=TRUE`** then

$$\mathrm{df} = \mathrm{length(knots)} + \mathrm{degree} + 1$$

- If you prefer to specify the degrees of freedom, then the function `bs()` chooses `df-degree` many knots at suitable quantiles of x (ignoring any missing values). If you specified `intercept=TRUE`, then the number of knots will be `df-degree-1`. For example,

Defining `knots` location in `bs()`

```
x=seq(0, 1, by=0.01) # generic `x` for illustration purposes
Bsplines.basis2 = bs(x, df=4)
head(Bsplines.basis2)
```

```
##              1        2        3 4
## [1,] 0.000000 0.000000 0.000000 0
## [2,] 0.058214 0.000592 0.000002 0
## [3,] 0.112912 0.002336 0.000016 0
## [4,] 0.164178 0.005184 0.000054 0
## [5,] 0.212096 0.009088 0.000128 0
## [6,] 0.256750 0.014000 0.000250 0
```

As an example, below we plot the first 7 B Splines basis functions:

Illustration of B Splines Basis Function

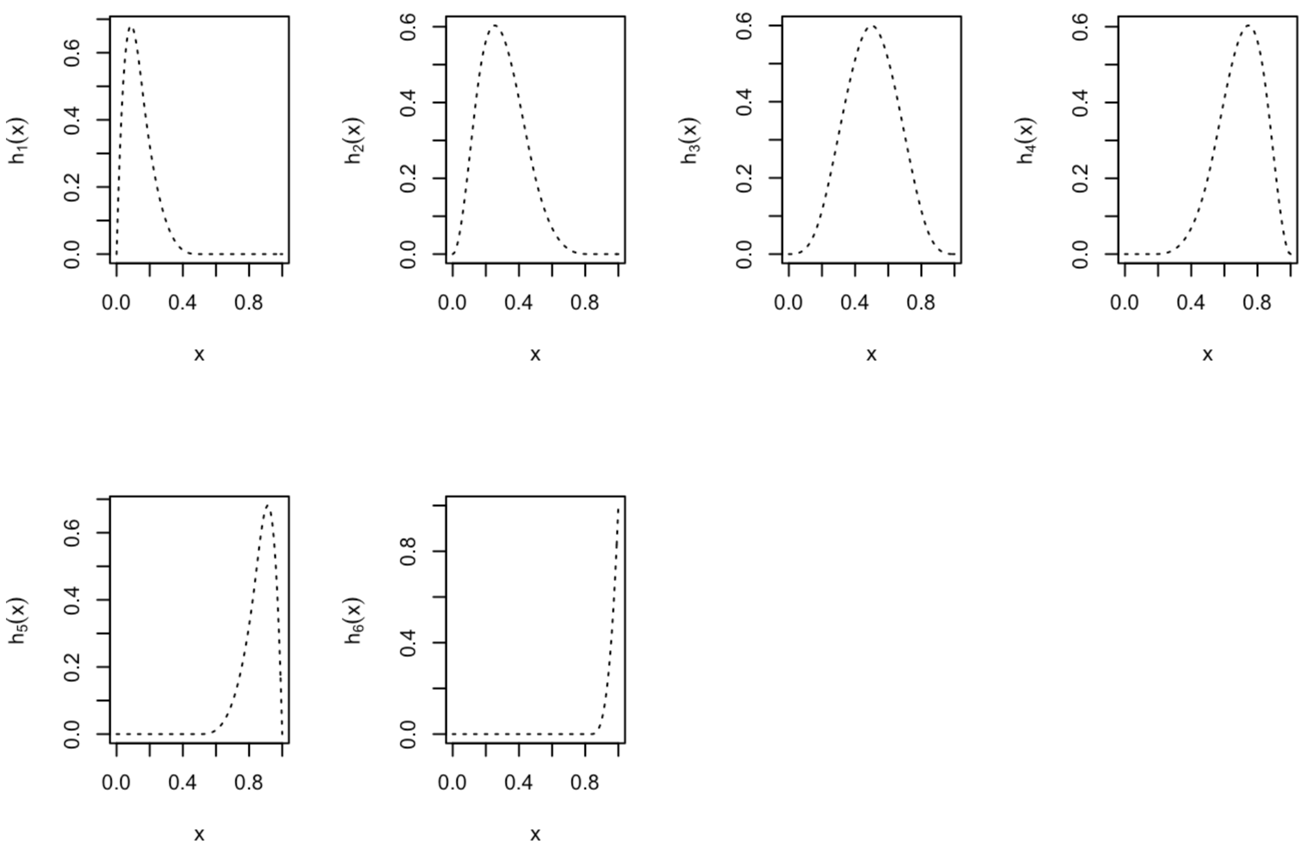
```
Bsplines.basis = bs(x, knots=new.knots)
dim(Bsplines.basis)
```

```
## [1] 101   6
```

```
head(Bsplines.basis)
```

```
##              1         2         3 4 5 6
## [1,] 0.000000 0.0000000 0.0000000 0 0 0
## [2,] 0.165912 0.0034896 0.0000144 0 0 0
## [3,] 0.304896 0.0135168 0.0001152 0 0 0
## [4,] 0.418824 0.0294192 0.0003888 0 0 0
## [5,] 0.509568 0.0505344 0.0009216 0 0 0
## [6,] 0.579000 0.0762000 0.0018000 0 0 0
```

```
par(mfrow = c(2,4))
plot(x, Bsplines.basis[,1], type='l', lty=3, ylab=expression(paste(h[1](x))))
plot(x, Bsplines.basis[,2], type='l',lty=3, ylab=expression(paste(h[2](x))))
plot(x, Bsplines.basis[,3], type='l',lty=3, ylab=expression(paste(h[3](x)) ))
plot(x, Bsplines.basis[,4], type='l',lty=3, ylab=expression(paste(h[4](x))))
plot(x, Bsplines.basis[,5], type='l',lty=3, ylab=expression(paste(h[5](x))))
plot(x, Bsplines.basis[,6], type='l',lty=3, ylab=expression(paste(h[6](x))))
```



4.5.3 Natural Cubic Splines (NCS)

A cubic spline on $[a, b]$ is a **Natural Cubic Spline** if its *second* and *third* derivatives are *zero at* a *and* b. This condition implies that NCS is a linear function in the two extreme intervals $[a, \xi_1]$ and $[\xi_m, b]$. The linear functions in the two extreme intervals are completely determined by their neighboring intervals. The degrees of freedom of NCS's with m knots are:

$$4(m+1) - 3m - 4 = m$$

since we have 4 additional constraints.)

Remark:For a curve estimation problem with data $(x_i, y_i)_{i=1}^n$, if we put n knots at the n data points (assumed to be unique), then using NCS we obtain a smooth curve passing through **all** y's.

Natural Cubic Spline

A Natural Cubic Spline with m knots is represented by m basis functions, for example one such basis is given by

$$\begin{aligned} N_1(x) &= 1 \\ N_2(x) &= x \\ N_{k+2}(x) &= d_k(x) - d_{k-1}(x) \end{aligned}$$

where

$$d_k(x) = \frac{(x - \xi_k)_+^3 - (x - \xi_m)_+^3}{\xi_m - \xi_k}$$

Each of these derivatives can be seen to have zero second and third derivative for $x \geq \xi_m$.

In `R` we can find the NCS as part of the `splines` library, by calling the `ns()` function. Specifically, we have that

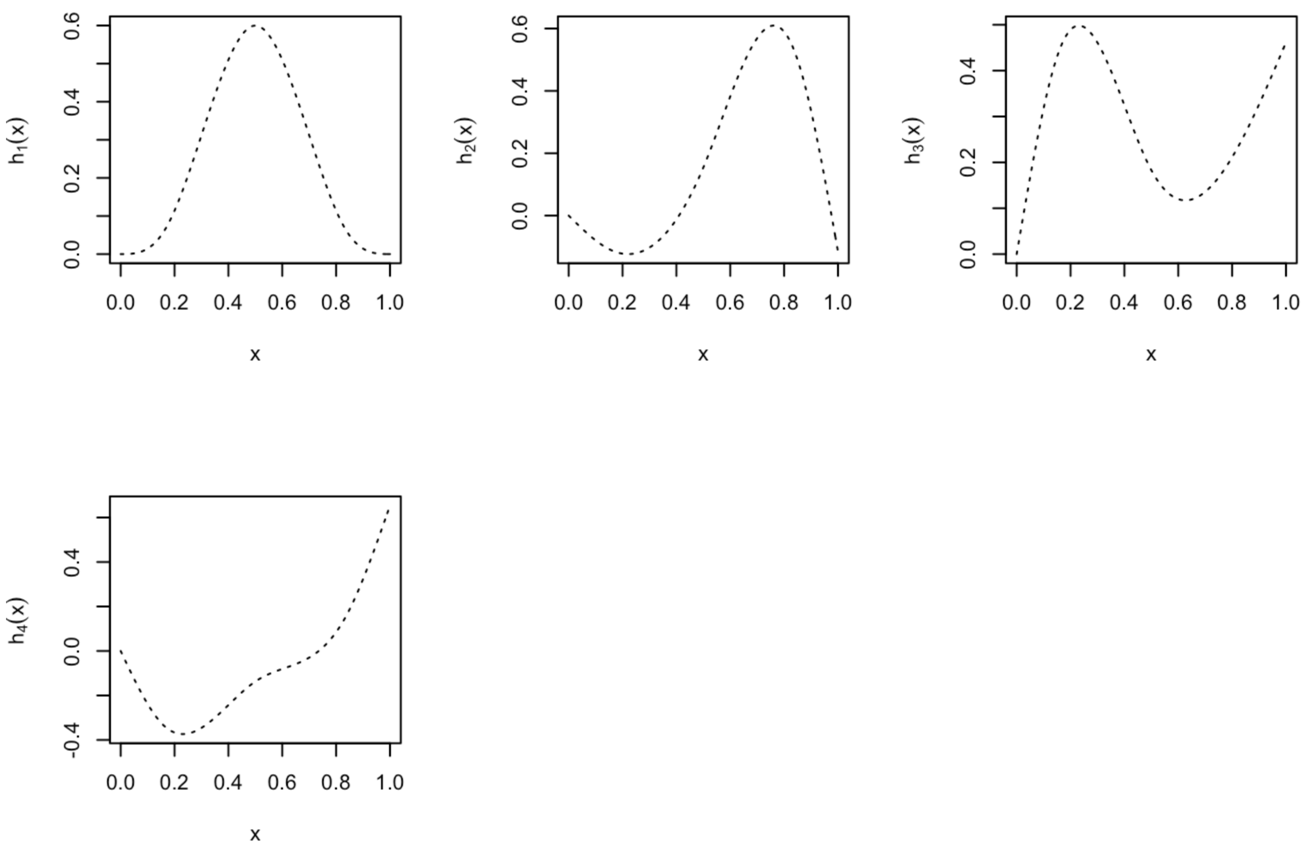
$$ns(x, df, knots, intercept = TRUE, Boundary.knots)$$

Natural Cubic Splines in `R`

```
NCS.basis =ns(x, knots=new.knots, Boundary.knots=c(0,1))
dim(NCS.basis)
```

```
## [1] 101   4
```

```
par(mfrow = c(2,3))
plot(x, NCS.basis[,1], type='l', lty=3, ylab=expression(paste(h[1](x))))
plot(x, NCS.basis[,2], type='l',lty=3, ylab=expression(paste(h[2](x))))
plot(x, NCS.basis[,3], type='l',lty=3, ylab=expression(paste(h[3](x)) ))
plot(x, NCS.basis[,4], type='l',lty=3, ylab=expression(paste(h[4](x))))
```



Recall that the linear functions in the two extreme intervals are completely determined by the other cubic splines. This means that data points in the two extreme intervals (i.e., outside the two boundary knots) are wasted since they do not affect the fitting. Therefore, by default, `R` puts the two boundary knots as the *min* and *max* of the x_i's.

As in the case of the `bs()` function:

- You can tell `R` the location of knots, which are the interior knots. Recall that a NCS with m knots has m df. So, the df is equal to the number of (interior) knots plus 2, where 2 means the two boundary knots.
- Or you can tell `R` the df. If intercept = TRUE, then we need $m = df - 2$ knots, otherwise we need $m = df - 1$ knots. Again, by default, `R` puts knots at the $1/(m+1), \ldots, m/(m+1)$ quantiles of $x_{1:n}$.

4.5.4 Regression Splines

Recall that for a given set of knots, the corresponding cubic splines form a *linear space* of functions with dimension $(m+4)$. So, the **Regression Splines** use a basis expansion approach:

$$g(x) = \beta_1 h_1(x) + \beta_2 h_2(x) + \ldots + \beta_p h_p(x)$$

* If Cubic Splines are used as basis functions $p = m + 4$.

- If Natural Cubic Splines (NCS) are used as basis functions $p = m$.

We can represent the model on the observed n data points using matrix notation:

$$\begin{pmatrix} y_1 \\ y_2 \\ \ldots \\ y_n \end{pmatrix}_{n\times 1} = \begin{pmatrix} h_0(x_1) & h_1(x_1) & \ldots & h_{p-1}(x_1) \\ h_0(x_2) & h_1(x_2) & \ldots & h_{p-1}(x_2) \\ & & & \\ h_0(x_n) & h_1(x_n) & \ldots & h_{p-1}(x_n) \end{pmatrix}_{n\times p} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \ldots \\ \beta_p \end{pmatrix}_{p\times 1}$$

where our *"design"* matrix is the matrix $\mathbf{F}$ of basis functions.

Therefore, we can estimate the coefficients β by solving the following Least-Squares problem:

$$\hat{\beta} = \arg\min_{\beta} ||\mathbf{y} - \mathbf{F}\beta||^2$$

Regression Splines in `R`

We can obtain the design matrix $\mathbf{F}$ by commands `bs` (B-splines) or `ns` (NCS) in `R`, and then call the regression function `lm` as shown in the following example:

Pumpkins Data Set

We start by fitting a model with B-splines and `df=5`. Note that we choose `intercept=FALSE` (the default) inside the `bs` function, because an intercept will be automatically added by the `lm` function. If we choose `intercept=TRUE`, then R will not be able to estimate two intercepts and will output NAs .

```
library(splines)
pumpkins.bs = lm(size ~ bs(price, df=5, intercept=FALSE), data=pumpkins)
summary(pumpkins.bs)
```

```
##
## Call:
## lm(formula = size ~ bs(price, df = 5, intercept = FALSE), data = pumpkins)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1.40250 -0.49560 -0.06913  0.48870  1.94349
##
## Coefficients:
##                                        Estimate Std. Error t value Pr(>|t|)
## (Intercept)                             0.51654    0.09964   5.184 4.59e-07 ***
## bs(price, df = 5, intercept = FALSE)1 -0.19979    0.16744  -1.193  0.23397
## bs(price, df = 5, intercept = FALSE)2  7.39369    0.54755  13.503  < 2e-16 ***
## bs(price, df = 5, intercept = FALSE)3 -1.34647    0.51698  -2.604  0.00977 **
## bs(price, df = 5, intercept = FALSE)4  2.79392    0.26166  10.677  < 2e-16 ***
## bs(price, df = 5, intercept = FALSE)5  2.55259    0.24564  10.392  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.6846 on 242 degrees of freedom
## Multiple R-squared:  0.7164, Adjusted R-squared:  0.7105
## F-statistic: 122.3 on 5 and 242 DF,  p-value: < 2.2e-16
```

```
dim(bs(pumpkins$price, df=5, intercept=FALSE))
```

```
## [1] 248   5
```

Of course, instead of B-splines, we can also choose to work with NCS. This can be done as follows:

```
pumpkins.ncs1 = lm(size ~ ns(price, knots=quantile(price, (1:4)/5)), data=pumpkir
summary(pumpkins.ncs1)
```

```
##
## Call:
## lm(formula = size ~ ns(price, knots = quantile(price, (1:4)/5)),
##     data = pumpkins)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -1.3249 -0.4706 -0.1105  0.5297  1.8704
##
## Coefficients:
##                                               Estimate Std. Error t value
## (Intercept)                                    0.46916    0.09119   5.145
## ns(price, knots = quantile(price, (1:4)/5))1  6.69572    0.60959  10.984
## ns(price, knots = quantile(price, (1:4)/5))2  1.20188    0.37175   3.233
## ns(price, knots = quantile(price, (1:4)/5))3  1.74531    0.16433  10.621
## ns(price, knots = quantile(price, (1:4)/5))4  2.35882    0.27024   8.729
## ns(price, knots = quantile(price, (1:4)/5))5  2.78451    0.23021  12.096
##                                               Pr(>|t|)
## (Intercept)                                   5.54e-07 ***
## ns(price, knots = quantile(price, (1:4)/5))1  < 2e-16 ***
## ns(price, knots = quantile(price, (1:4)/5))2   0.0014 **
## ns(price, knots = quantile(price, (1:4)/5))3  < 2e-16 ***
## ns(price, knots = quantile(price, (1:4)/5))4 4.28e-16 ***
## ns(price, knots = quantile(price, (1:4)/5))5  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.6942 on 242 degrees of freedom
## Multiple R-squared:  0.7084, Adjusted R-squared:  0.7024
## F-statistic: 117.6 on 5 and 242 DF,  p-value: < 2.2e-16
```

```r
dim(ns(pumpkins$price, knots=quantile(pumpkins$price, (1:4)/5)))
```

```
## [1] 248   5
```

In the example above, we arbitrarily chose the number of knots and/or the degrees of freedom in the splines expansion. So, a natural question that arises here is: what is the right number of knots or degrees of freedom for our problem?

To answer this question, we will use what we call K-fold cross-validation (CV).

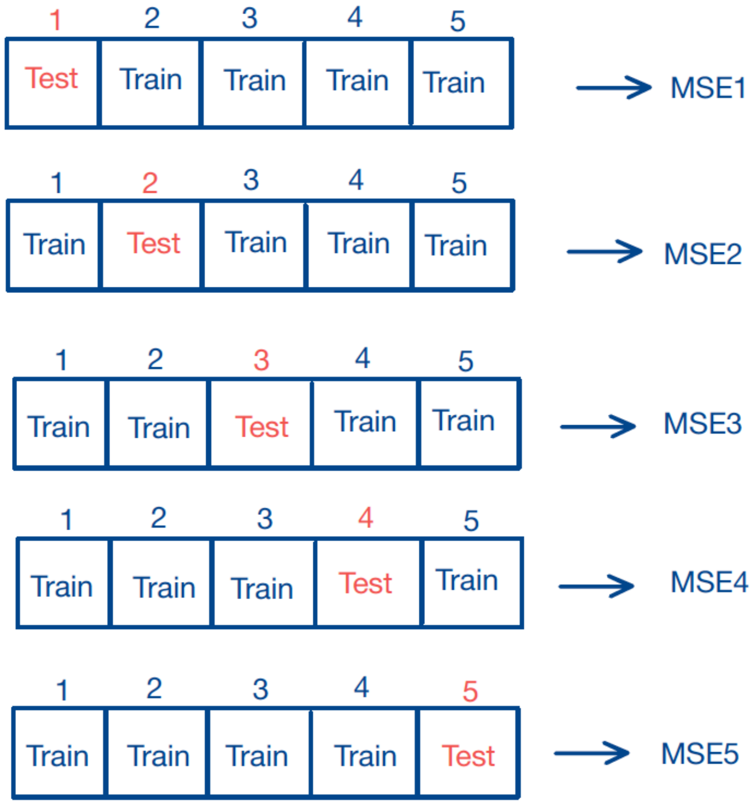
4.5.5 K-Fold Cross-Validation

How to select the optimal number of knots (or df)? The process is the following:

K-Fold Cross-Validation

1. Set a fixed number of knots (or df).
2. Divide the set of observations into k groups (or folds).
3. Leave the first fold as a validation set (not used to fit the model). Fit the Regression Spline with a fixed number of knots using the remaining $k-1$ folds.
4. Calculate the Mean Square Error for fold 1: MSE_1.
5. Repeat the previous steps k times. Each time a new validation set is used to calculate MSE_i.
6. Calculate the average k-fold Cross-Validation error: $CV(k) = \frac{1}{k}\sum_{i=1}^{k} MSE_i$.
7. Repeat 2 to 6 with a new number of knots (or df).
8. Select the number of knots that minimizes the k-fold CV error or $CV(k)$.

This process is also summarized in the following sketch:



$$\overline{\frac{1}{k}\sum_{i=1}^{k} MSE_i}$$

K- Fold Cross Validation Error

Pumpkins Data Set

```
library(caret)

  CV_K =c() # initialize the vector to store the CV(k) errors for every fixed kr

  for (knots in 3:7) {  # we start with 3 knots and go up to 7 knots

   j=knots-2 # counter index starting at 1
   MSE_i = c()

   for (k in 3:10){   # loop over the number of folds in the data
     i=k-2 # counter index starting at 1
     folds <- createFolds(pumpkins$price, k) # Create the folds

     # Function that fits the model,  computes the MSE of every fold
     results = lapply(folds, function(x){
       pumpkin_train = pumpkins[-x,] # Create train set for fold "x"
       pumpkin_test = pumpkins[x,] # Create corresponding test set.
       pumpkins.bs = lm(size ~ bs(price, knots, intercept=FALSE), data=pumpkin_t
       pumpkin.pred = predict(pumpkins.bs, newdata=pumpkin_test) # Test the mode
       mserror = mean( (pumpkin_test$size-pumpkin.pred)^2) # Compute the MSEi fc
       return(mserror)
    })
    MSE_i[i] = mean(unlist(results))  # Repeat the previous steps k times
   }

   CV_K[j] = mean(MSE_i) # This is the CV_k for j+2 knots
 }

  CV_K
```

```
## [1] 0.5214599 0.4956015 0.4739036 0.4720174 0.4657793
```

```
NumberOfKnots = which.min(CV_K) +2
NumberOfKnots
```

```
## [1] 7
```