Michael Leibert Math 504 Homework 10

2. Consider $f(x) = e^x$. Note that f'(0) = 1. Consider the following two finite differences:

$$\frac{f(x+h) - f(x)}{h}. (1)$$

$$\frac{f(x+h) - f(x-h)}{2h}. (2)$$

For $h = 10^i$ with $i = -20, -19, -18, \ldots, -1, 0$ calculate both finite differences. For each h, determine how many digits in the finite difference estimate are correct (you know the true value of the derivative is 1). Note that .99991 is correct up to 4 digits since .999999 $\cdots = 1$. Explain your results given finite differences and floating point error. DON'T FORGET TO SET options(digits=16).

```
options(scipen=999); options(digits=15)
f<-function(x) {exp(x)}

x=0; i=0:-20; h=10^i
a<- (( f(x + h) - f(x) ) / h )

dat<-data.frame(paste0("10^",i),a)</pre>
```

```
b < - (f(x + h) - f(x-h)) / (2*h)
dat$b<-b
```

```
##
       10^i
                              accuracy
                                                        bccuracy
## 1
                                                              0
       10^0 1.718281828459045
                                    0 1.175201193643801
                                                              2
## 2
      10^-1 1.051709180756477
                                    1 1.001667500198441
## 3
      10^-2 1.005016708416795
                                    2 1.000016666749992
                                                              4
                                                              6
      10^-3 1.000500166708385
                                    3 1.000000166666681
## 4
## 5
      10^-4 1.000050001667141
                                    4 1.00000001666890
                                                              8
## 6
      10^-5 1.000005000006965
                                    5 1.00000000012102
                                                              10
## 7
      10^-6 1.000000499962184
                                    6 0.99999999973245
                                                              10
## 8
      10^-7 1.000000049433680
                                    7 0.99999999473644
                                                              9
## 9
      10^-8 0.99999993922529
                                    8 0.99999993922529
                                                              8
## 10 10^-9 1.000000082740371
                                                              7
                                    7 1.000000027229220
## 11 10^-10 1.000000082740371
                                    7 1.000000082740371
                                                              7
                                                              7
## 12 10^-11 1.000000082740371
                                    7 1.000000082740371
## 13 10^-12 1.000088900582341
                                    4 1.000033389431110
                                                              4
## 14 10^-13 0.999200722162641
                                    3 0.999755833674953
                                                              3
## 15 10^-14 0.999200722162641
                                                              3
                                    3 0.999200722162641
## 16 10^-15 1.110223024625157
                                    0 1.054711873393899
                                                               1
## 17 10^-16 0.0000000000000000 inaccurate 0.555111512312578 inaccurate
## 18 10^-17 0.00000000000000000000 inaccurate 0.000000000000000 inaccurate
## 19 10^-18 0.0000000000000000 inaccurate 0.00000000000000 inaccurate
```

We can see the inherent trade-off here. For small values of h we run into floating point errors that are blown up. We see this for the i's from 14 to 20. However, for large values of h, our approximation to the derivative suffers. We see this in the first 5-6 rows where the level of accuracy is under 5 places, especially in the first column. For finite difference (2), the first-order errors cancel and has an additional expansion in the Taylor's Series. Relative to finite difference (1), for small values of h this generates a more accurate approximation to the derivative.

3. Consider the following finite difference

$$Df_h(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}.$$
 (3)

This finite difference is used to estimate f''(x). Calculate the error of this approximation in terms of h and machine epsilon.

error =
$$\left| \frac{f\ell(f(x_0+h)) - f\ell(2f(x_0)) + f\ell(f(x_0-h))}{h^2} - f''(x_0) \right|$$

$$= \left| \frac{f(x_0+h)(1+\epsilon_1) - 2f(x_0)(1+\epsilon_2) + f(x_0-h)(1+\epsilon_1)}{h^2} - f''(x_0) \right|$$

$$= \left| \frac{f(x_0+h)\epsilon_1 - 2f(x_0)\epsilon_2 + f(x_0-h)\epsilon_3}{h^2} + \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2} - f''(x_0) \right|$$

$$= \left| \frac{c \cdot 10^{-16}}{h^2} + \left(\frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2} - f''(x_0) \right) \right|$$

Note for i = 1, 2, 3 the $|\epsilon_i| \le 10^{-16}$. We perform the Taylor series expansion of $f(x_0 + h)$ and $f(x_0 - h)$.

$$f(x_0 + h) \approx f(x_0) + f'(x_0) \cdot h + \frac{1}{2} f''(x_0)h^2 + \frac{1}{6} f'''(x_0)h^3 + \frac{1}{4!} f^{(4)}(x_0)h^4$$

$$f(x_0 - h) \approx f(x_0) - f'(x_0) \cdot h + \frac{1}{2} f''(x_0)h^2 - \frac{1}{6} f'''(x_0)h^3 + \frac{1}{4!} f^{(4)}(x_0)h^4$$

$$\text{error} = \left| \frac{c \cdot 10^{-16}}{h^2} + \left(\frac{f(x_0) + f'(x_0) \cdot h + \frac{1}{2} f''(x_0)h^2 + \frac{1}{4!} f'^{(4)}(x_0)h^4 - 2f(x_0) + f(x_0) - f'(x_0) \cdot h + \frac{1}{2} f''(x_0)h^2 - \frac{1}{6} f'''(x_0)h^3 + \frac{1}{4!} f^{(4)}(x_0)h^4 - 2f(x_0) + f(x_0) - f'(x_0) \cdot h + \frac{1}{2} f''(x_0)h^2 - \frac{1}{6} f'''(x_0)h^3 + \frac{1}{4!} f^{(4)}(x_0)h^4 - 2f(x_0) - \frac{1}{6} f'''(x_0)h^4 - \frac{1}{6} f'''(x_0)h^4$$

We seek to minimize this quantity, so we take the derivative in h and set it equal to zero

$$0 = -\frac{2c \cdot 10^{-16}}{h^3} + \frac{h}{6} f^{(4)}(x_0)$$

$$\frac{2c \cdot 10^{-16}}{h^3} = \frac{h}{6} f^{(4)}(x_0)$$

$$h^4 = \frac{12c \cdot 10^{-16}}{|f^{(4)}(x_0)|}$$

$$h = \left(\frac{12c \cdot 10^{-16}}{|f^{(4)}(x_0)|}\right)^{\frac{1}{4}}$$
error $\simeq 10^{-4}$

4. The file **BoneMassData.txt** contains bone mass data for men and women at a variety of ages. This data comes from the book, "The Elements of Statistical Learning". In this problem, we will apply a spline regression to the dataset using predetermined knots. Specifically our regression model will be $y \sim S(x)$ were x is the age, y is the bone mass, and S(x) is a cubic spline. For brevity consider only the samples taken from women and for simplicity consider two knots with $\xi_1 = 15$ and $\xi_2 = 20$ (the case of more knots is no different). Then our splines are determined by the parameters a_i, b_i, c_i, d_i for i = 0, 1, 2 where $S_i(x) = a_i + b_i x + c_i x^2 + d_i x^3$ and

$$S(x) = \begin{cases} S_0(x) & \text{if } x < \xi_1 \\ S_1(x) & \text{if } x \in [\xi_1, \xi_2) \\ S_2(x) & \text{if } x \ge \xi_2, \end{cases}$$

with the requirement that S(x), S'(x), S''(x) be continuous at the two knots. Our goal is to find S(x) that minimizes the sum of squared residuals

$$\sum_{i=1}^{N} (y_i - S(x_i))^2,$$

where (x_i, y_i) are the datapoints.

(a) Suppose that we can decompose any cubic spline S(x) with knots at $\xi = 15, 20$ as a linear combination of the functions $h_1(x), h_2(x), \ldots, h_D(x)$ for some D. That is, any cubic spline with knots at ξ_1, ξ_2 can be written as

$$S(x) = \sum_{j=1}^{D} \alpha_i h_i(x)$$

Show that the spline S(x) that minimizes the sum of squared residuals is given by α defined by $\alpha = (B^TB)^{-1}B^Ty$ where y is the vector of y_i values and B is a $N \times D$ matrix given by $B_{k\ell} = h_{\ell}(x_k)$. (We did this in class, I want you to go through the details.)

We define our linear function space as

$$\mathcal{F} = \{S(x) : S(x) \text{ is a cubic spline with knots at } \zeta_1 \text{ and } \zeta_2\}$$

Our desire is to:

$$\min_{S(x)\in\mathcal{F}} \sum_{i=1}^{N} \left| y_i - S\left(x^{(i)}\right) \right|^2$$

where,

$$S(x^{(i)}) = \sum_{i=1}^{D} \alpha_{j} h_{j}(x) = \alpha_{1} h_{1}(x) + \alpha_{2} h_{2}(x) + \dots + \alpha_{D} h_{D}(x).$$

$$\min_{S\left(x\right)\in\mathcal{F}}\sum_{i=1}^{N}\left|y_{i}-s\left(x^{\left(i\right)}\right)\right|^{2}=\min_{\alpha\in\mathbb{R}^{D}}\sum_{i=1}^{N}\left|y_{i}-\alpha_{1}h_{1}\left(x\right)-\alpha_{2}h_{2}\left(x\right)-\ldots-\alpha_{D}h_{D}\left(x\right)\right|^{2}.$$

We can write the difference contained within the absolute value in matrix form:

Instead of writing the minimization as a large sum, we can write

$$\min_{s(x)\in\mathcal{F}} \sum_{i=1}^{N} \left| y_i - s\left(x^{(i)}\right) \right|^2 = \min_{\alpha\in\mathbb{R}^D} \sum_{i=1}^{N} \left| y_i - \alpha_1 h_1\left(x^{(i)}\right) - \alpha_2 h_2\left(x^{(i)}\right) - \dots - \alpha_D h_D\left(x^{(i)}\right) \right|^2 \qquad (4)$$

$$= \min_{\alpha\in\mathbb{R}^D} \left| |\mathbf{y} - B\boldsymbol{\alpha}| \right|^2$$

The solution to (5) can be solved with the normal equations, $\alpha = (B^T B)^{-1} B^T \mathbf{y}$.

(b) Now show that D from (a) has value D = 6. (Again, we did this in class.)

If there are no continuity conditions we can take any 12 dimensional vector to represent our spline.

$$\bar{S}(x) \in \mathcal{F} \Longleftrightarrow \begin{pmatrix} a_1 \\ b_1 \\ c_1 \\ \vdots \\ d_3 \end{pmatrix}$$

$$12 \times 1$$

This is a one to one mapping. If given a spline in \mathcal{F} then that corresponds to a 12 dimensional vector. And if given all the a's, b's, c's, and d's then that specifies the spline.

If we have an another vector $\hat{S}(x) \in \mathcal{F} \iff \begin{pmatrix} \hat{a}_1 \\ \hat{b}_1 \\ \hat{c}_1 \\ \vdots \\ \hat{d}_3 \end{pmatrix}$ and we linearly combine it with $\bar{S}(x)$.

$$e_{1}\bar{S}(x) + e_{2}\hat{S}(x) \iff \begin{pmatrix} e_{1}a_{1} + e_{2}\hat{a}_{1} \\ e_{1}b_{1} + e_{2}\hat{b}_{1} \\ e_{1}c_{1} + e_{2}\hat{c}_{1} \\ \vdots \\ e_{1}d_{3} + e_{2}\hat{d}_{3} \end{pmatrix}$$

$$12 \times 1$$

The linear combination will also be in \mathcal{F} .

However, we wish to enforce the continuity conditions. To enforce the continuity conditions, we set up the following system of equations:

$$\begin{cases} S_0(\zeta_1) = S_1(\zeta_1) \\ S'_0(\zeta_1) = S'_1(\zeta_1) \\ S''_0(\zeta_1) = S''_1(\zeta_1) \\ S_1(\zeta_2) = S_2(\zeta_2) \\ S'_1(\zeta_2) = S'_2(\zeta_2) \\ S''_1(\zeta_2) = S''_2(\zeta_2) \end{cases}$$

If we want the 12 dimensional vector to represent a spline, meaning it gives us the coefficients $a_1, b_1, ..., d_3$ that will build us a spline that has continuity conditions, we need $M\mathbf{v} = 0$. We can put the conditions in matrix form, with the requirement that each of the continuity conditions hit zero:

$$\begin{pmatrix} 1 & \zeta_1 & \zeta_1^2 & \zeta_1^3 & -1 & -\zeta_1 & -\zeta_1^2 & -\zeta_1^3 & 0 & 0 & 0 & 0 \\ 0 & 1 & 2\zeta_1 & 3\zeta_1^2 & 0 & -1 & -2\zeta_1 & -3\zeta_1^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 6\zeta_1 & 0 & 0 & -2 & -6\zeta_1 & 0 & 0 & 0 & 0 \\ & & & & \vdots & & & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 6\zeta_2 & 0 & 0 & -2 & -6\zeta_2 \end{pmatrix} \begin{pmatrix} a_1 \\ b_1 \\ c_1 \\ d_1 \\ \vdots \\ d_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Where M is 6×12 and \mathbf{v} is 12×1 . The space of all 12 dimensional vectors such that $M\mathbf{v} = \mathbf{0}$ is the kernel, another linear space.

We can now find $D = \dim(\mathcal{F})$. Using the theorem, if M is an $n \times k$ matrix with k > n, then $\dim(\ker(m)) = k - n$, where $n = \dim(\operatorname{range}(m))$. So D = 12 - 6 = 6

(c) Show that the six functions $h_1(x) = 1$, $h_2(x) = x$, $h_3(x) = x^2$, $h_4(x) = x^3$, $h_5(x) = [x - \xi_1]_+^3$, $h_6(x) = [x - \xi_2]_+^3$ form a basis for all splines with knots at $\xi = 15, 20$. To do this you must show (i) each $h_i(x)$ is a spline for the two knots, (ii) each spline must be a linear combination of these functions and (iii) the $h_i(x)$ cannot be linearly combined to give the zero function.

We show each $h_i(x)$ is a spline for the two knots.

$$h_1(x) = 0x^3 + 0x^2 + 0x + 1x^0 = 1$$
 $h_2(x) = 0x^3 + 0x^2 + 1x + 0x^0 = x$ $h_3(x) = 0x^3 + 1x^2 + 0x + 0x^0 = x^2$ $h_4(x) = 1x^3 + 0x^2 + 0x + 0x^0 = x^3$

For i = 1, 2, 3, 4, h_i are cubic polynomials $\forall x$ and are splines for the two knots and have a continuous second derivative.

For $h_5(x) = [x - \zeta_1]_+^3$ it is a cubic polynomial for $x \in [\zeta_1, \infty)$ and for $h_6(x) = [x - \zeta_2]_+^3$ it is a cubic polynomial for $x \in [\zeta_2, \infty)$ and are both are splines for the two knots.

Since $h_5(x)$ is a cubic polynomial in the range $[\zeta_1, \infty)$ it, along with its first and second derivatives, is continuous across ζ_1 and ζ_2 . Likewise, Since $h_6(x)$ is a cubic polynomial in the range $[\zeta_2, \infty)$ it, along with its first and second derivatives, is continuous across ζ_1 and ζ_2 .

We check for continuity across ζ_1 and ζ_2 for the functions h_5 and h_6 .

 $h_5(x)$ continuous across ζ_1 :

$$\lim_{x \to \zeta_1^-} h_5(x) = \lim_{x \to \zeta_1^-} 0 = 0$$
$$\lim_{x \to \zeta_1^+} h_5(x) = \lim_{x \to \zeta_1^+} [x - \xi_1]^3 = 0$$
$$h_5(\zeta_1) = 0$$

 $h_5(x)$ continuous across ζ_2 :

$$\lim_{x \to \zeta_2^-} h_5(x) = \lim_{x \to \zeta_2^+} h_5(x) = h_5(\zeta_2) = (\zeta_2 - \zeta_1)^3$$

 $h_5'(x)$ continuous across ζ_1 :

$$\lim_{x \to \zeta_1^-} h_5'(x) = \lim_{x \to \zeta_1^-} 0 = 0$$
$$\lim_{x \to \zeta_1^+} h_5'(x) = \lim_{x \to \zeta_1^+} 3(x - \zeta_1)^2 = 0$$
$$h_5'(\zeta_1) = 0$$

 $h_5'(x)$ continuous across ζ_2 :

$$\lim_{x \to \zeta_2^-} h_5'(x) = \lim_{x \to \zeta_2^+} h_5'(x) = h_5'(\zeta_2) = 3(\zeta_2 - \zeta_1)^2$$

 $h_5''(x)$ continuous across ζ_1 :

$$\lim_{x \to \zeta_1^-} h_5''(x) = \lim_{x \to \zeta_1^-} 0 = 0$$

$$\lim_{x \to \zeta_1^+} h_5''(x) = \lim_{x \to \zeta_1^+} 3(x - \zeta_1)^2 = 0$$

$$h_5''(\zeta_1) = 0$$

 $h_5''(x)$ continuous across ζ_2 :

$$\lim_{x \to \zeta_2^-} h_5''(x) = \lim_{x \to \zeta_2^+} h_5''(x) = h_5''(\zeta_2) = 6(\zeta_2 - \zeta_1)$$

 $h_6(x)$ continuous across ζ_1 :

$$\lim_{x \to \zeta_1^-} h_6(x) = \lim_{x \to \zeta_1^+} h_6(x) = h_6(\zeta_1) = 0$$

 $h_6(x)$ continuous across ζ_2 :

$$\lim_{x \to \zeta_2^-} h_6(x) = \lim_{x \to \zeta_2^-} 0 = 0$$
$$\lim_{x \to \zeta_2^+} h_6(x) = \lim_{x \to \zeta_2^+} (x - \zeta_2)^3 = 0$$
$$h_6(\zeta_2) = 0$$

 $h_6'(x)$ continuous across ζ_1 :

$$\lim_{x \to \zeta_1^-} h_6'(x) = \lim_{x \to \zeta_1^+} h_6'(x) = h_6'(\zeta_1) = 0$$

 $h_{6}^{'}(x)$ continuous across ζ_{2} :

$$\lim_{x \to \zeta_2^-} h_6'(x) = \lim_{x \to \zeta_2^-} 0 = 0$$

$$\lim_{x \to \zeta_2^+} h_6'(x) = \lim_{x \to \zeta_2^+} 3(x - \zeta_2)^2 = 0$$

$$h_6'(\zeta_2) = 0$$

 $h_6''(x)$ continuous across ζ_1 :

$$\lim_{x \to \zeta_1^-} h_6''(x) = \lim_{x \to \zeta_1^+} h_6''(x) = h_6''(\zeta_1) = 0$$

 $h_6''(x)$ continuous across ζ_2 :

$$\lim_{x \to \zeta_2^-} h_6''(x) = \lim_{x \to \zeta_2^-} 0 = 0$$

$$\lim_{x \to \zeta_2^+} h_6''(x) = \lim_{x \to \zeta_2^+} 6(x - \zeta_2) = 0$$

$$h_6'(\zeta_2) = 0$$

We now show that each spline is a linear combination of these functions.

Consider the first region, $(-\infty, \zeta_1]$. $h_5(x)$ and $h_6(x)$ are 0 here, so we can match the function S_0 exactly if we choose a_0, b_0, c_0, d_0 .

$$S_0(x) = a_0 h_1(x) + b_0 h_2(x) + c_0 h_3(x) + d_0 h_4(x) = a_0 + b_0 x + c_0 x^2 + d_0 x^3$$

For the second region, $[\zeta_1, \zeta_2]$, choose a coefficient e for $h_5(x)$. Recall $h_6(x)$ is 0 here. Then in the second region we have:

$$ah_1(x) + bh_2(x) + ch_3(x) + dh_4(x) + eh_5(x)$$

$$= a + bx + cx^2 + dx^3 + e(x - \zeta_1)^3$$

$$= (d + e)x^3 + (c - 3e\zeta_1)x^2 + (b + 3e\zeta_1^2)x + (a - e\zeta_1^3)$$

 ζ_1 is fixed so if we pick the correct a, b, c, d, e to we can match S_1 exactly.

Similarly, for the last region we can repeat this process. The third region $[\zeta_2, \infty)$, all functions are defined, so choose a coefficient e for $h_5(x)$ and f for $h_6(x)$

$$ah_1(x) + bh_2(x) + ch_3(x) + dh_4(x) + eh_5(x) + fh_6(x)$$

$$= a + bx + cx^2 + dx^3 + e(x - \zeta_1)^3 + f(x - \zeta_2)^3$$

$$= (d + e + f)x^3 + (c - 3e\zeta_1 - 3f\zeta_2)x^2 + (b + 3e\zeta_1^2 + 3f\zeta_2^2)x + (a - e\zeta_1^3 - f\zeta_2^3)$$

 ζ_1 and ζ_2 are fixed so if we pick the correct a, b, c, d, e, f to we can match S_2 exactly.

To show that the $h_i(x)$ cannot be linearly combined to give the zero function, we will test values in each region to ensure that our function is not the zero function. We note that in this linear function space, the 0 element is the function $z(x) = 0, \forall x$. We choose coefficients not all equal to zero, $\alpha = (-1.995, 0.4447, -0.0311, 0.0007, -0.0006, -0.0002)$

$$x = 10$$

$$-1.995 + 0.4447(10) - 0.0311(10)^{2} + 0.0007(10)^{3} - 0.0006(0) - 0.0002(0) = 0.042$$

$$x = 19$$

$$-1.995 + 0.4447(19) - 0.0311(19)^{2} + 0.0007(19)^{3} - 0.0006(19) - 0.0002(0) = 0.0285$$

$$x = 25$$

$$-1.995 + 0.4447(25) - 0.0311(25)^{2} + 0.0007(25)^{3} - 0.0006(25) - 0.0002(25) = 0.6225$$

In each region none of these functions is the zero function. Thus, because of this, along with the fact that each of the $h_i(x)$'s are splines for the two knots, and each spline is a linear combination of the $h_i(x)$'s, we can say that these six function form a basis for all spines with knots at $\zeta_1 = 15$ and $\zeta_2 = 20$.

(d) Now compute the regression spline S(x) and plot it along with the data points to show the fit. (Typically it is better to do the actual fitting using a call to \mathbf{lm} or using a spline regression package, but it's good to go through the process yourself at least once.)

```
bone<-read.table("BoneMassData.txt",header=T)
x=bone$age #£
y=bone[,4]
#model Matrix</pre>
```

```
B<-as.matrix(cbind(rep(1,485),x,x^2,x^3,ifelse(x<15,0,(x-15)^3),ifelse(x<20,0,(x-20)^3)))
a<-solve(t(B)%*%B)%*%t(B)%*%as.matrix(y)

#Regression Spline S(x)
Sx<-function(X){ a[1]*1 + a[2]*X+a[3]*X^2+a[4]*X^3+a[5]*
ifelse(X<15,0,(X-15)^3)+a[6]*ifelse(X<20,0,(X-20)^3) }

X<-seq(min(x), max(x), length = 485)

plot( bone$age,bone[ ,4])
lines( Sx(X) ~ X, lwd = 2, col = "blue")</pre>
```

