## CS 4210: Midterm Solution Guide

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| Problem 1 | 25 points | 18.8 |
| :--- | :--- | :--- |
| Problem 2 | 10 points | 5.9 |
| Problem 3 | 15 points | 14.8 |
| Problem 4 | 25 points | 17.6 |
| Problem 5 | 25 points | 19.1 |



Guidelines:

$$
85 \leq A \leq 100,65 \leq B \leq 80,45 \leq C \leq 60
$$

1. The second derivative rule

$$
D_{2}(f, a, h)=\frac{-f(a-2 h)+16 f(a-h)-30 f(a)+16 f(a+h)-f(a+2 h)}{12 h^{2}}
$$

has the property that

$$
f^{(2)}(a)=D_{2}(f, a, h)+c f^{(6)}(\eta) h^{4} \quad a-2 h \leq \eta \leq a+2 h
$$

where $c$ is a constant. For two separate examples (each with a known second derivative) we plot the value of $\left|f^{(2)}(a)-D_{2}(f, a, h)\right|$ for various values of $h$ and obtain the following:


The total error that is displayed in these plots is a combination of roundoff error and "math error". Model the total error as a function of $h$ and use it to explain the shape of the graphs and what determines the best value of $h$. Notice that the optimum $h$ values and the minimum error values are rather different in the two examples. Offer a possible explanation. Be brief! No proofs necessary.

You are to "model the total error as a function of $h$ " so anything of the form

$$
(\text { something })^{*} h^{4}+\text { something } / h^{2}
$$

is fine for 15 points, e.g.

$$
\operatorname{err}(h)=M_{6} h^{4}+\frac{\epsilon}{h^{2}}
$$

where $M_{6}$ captures some aspect of the size of $f^{(6)}$. Up to eight points for talking qualitatively about the model. Have to show that math error goes down with $h$ and rounding error goes up as $h$ decreases.

5 points for differentiating err and setting the result to zero. Will get something like $h_{o p t} \approx\left(\epsilon / M_{6}\right)^{1 / 6}$.
5 points for explaining why $h_{o p t}$ is different: best answer, the sixth derivative of the function in the second example is much bigger.
2. Assume that if the following script is run on a computer that implements 64 -bit IEEE floating point arithmetic, then it assigns the value of 53 to p

```
x = 1;
p = 0;
y = 1;
z = x +y ;
while z > x
    y = y/2;
    p = p + 1;
    z = x + y;
end
```

(a) What value is assigned to p if the first statement is changed to $\mathrm{x}=128$ ? Briefly justify your answer.

Note that in the given script

$$
z=1+1 / 2^{p}=\left(1+1 / 2^{p}\right) \times 2^{0}
$$

In the modified script

$$
z=128+1 / 2^{p}=\left(1+1 / 2^{p+7}\right) \times 2^{7}
$$

If the original script stops when $p=53$, then the modified one stops when $(p+7)=53$, i.e., when $p=46$. 5 points for this. Off-by-one answers OK too.
(b) Does the loop terminate if the first statement is changed to $\mathrm{x}=0$ ? Why?
$z=1 / 2^{p}=1.00 \times 2^{-} p$ Eventually there just are not enough bits in the exponent to represent p. 5 points for this. When this happens the result is set to zero. The loop terminates. It has nothing to do with the machine precision. Many thought if $z<e p s=2^{-53}$ then it is set to zero. Not true. This question is all about the exponent and has nothing to do with the mantissa.

Check out the lecture script FpFacts. In parts (a) and (b) minor points if you show some understanding of the finiteness of floating point representation, i.e., (mantissa part)*(power of 2) with limited hardare for each part.
3. Define the piecewise quadratic function $Q(x)$ by

$$
Q(x)= \begin{cases}q_{1}(x)=s_{1}+\left(y_{2}-y_{1}\right)\left(x-\frac{1}{2}\right)+2\left(y_{1}-2 s_{1}+y_{2}\right)\left(x-\frac{1}{2}\right)^{2} & 0 \leq x \leq 1 \\ q_{2}(x)=s_{2}+\left(y_{3}-y_{2}\right)\left(x-\frac{3}{2}\right)+2\left(y_{2}-2 s_{2}+y_{3}\right)\left(x-\frac{3}{2}\right)^{2} & 1 \leq x \leq 2\end{cases}
$$

It can be shown that $Q(0)=y_{1}, Q(1)=y_{2}$, and $Q(2)=y_{3}$ no matter how we choose the parameters $s_{1}$ and $s_{2}$. Thus, $Q(x)$ is a continuous interpolant of the points $\left(0, y_{1}\right),\left(1, y_{2}\right)$ and $\left(2, y_{3}\right)$. Show that it is possible to choose $s_{1}$ and $s_{2}$ so that $Q^{\prime}(x)$ is also continuous.

8 points for identifying this as the key equation: $q_{1}^{\prime}(1)=q_{2}^{\prime}(1)$
7 points for spelling it out

$$
\left(y_{2}-y_{1}\right)+4\left(y_{1}-2 s_{1}+y_{2}\right)\left(1-\frac{1}{2}\right)=\left(y_{3}-y_{2}\right)+4\left(y_{2}-2 s_{2}+y_{3}\right)\left(1-\frac{3}{2}\right)
$$

i.e.,

$$
\left(y_{2}-y_{1}\right)+2\left(y_{1}-2 s_{1}+y_{2}\right)=\left(y_{3}-y_{2}\right)-2\left(y_{2}-2 s_{2}+y_{3}\right)
$$

i.e.,

$$
s_{1}+s_{2}=\frac{y_{1}+6 y_{2}+y_{3}}{4}
$$

4. Define the cubic spline

$$
B_{*}(z)=\left\{\begin{array}{lr}
0 & z \leq-2 \\
(2+z)^{3} / 6 & -2 \leq z \leq-1 \\
\left(-3(1+z)^{3}+3(1+z)^{2}+3(1+z)+1\right) / 6 & -1 \leq z \leq 0 \\
\left(-3(1-z)^{3}+3(1-z)^{2}+3(1-z)+1\right) / 6 & 0 \leq z \leq 1 \\
(2-z)^{3} / 6 & 1 \leq z \leq 2 \\
0 & 2 \leq z
\end{array}\right.
$$

and note that

$$
B_{*}^{\prime \prime \prime}(z)=\left\{\begin{array}{rl}
0 & z<-2 \\
1 & -2<z<-1 \\
-18 & -1<z<0 \\
18 & 0<z<1 \\
-1 & 1<z<2 \\
0 & 2<z
\end{array}\right.
$$

Assume that $x_{k}=a+(k-1) h$ where $a$ and $h>0$ are given and define

$$
B_{k}(z)=B_{*}\left(\frac{z-x_{k}}{h}\right)
$$

for $k=0,1, \ldots, n+1$. If

$$
s(z)=\sum_{k=0}^{n+1} \alpha_{k} B_{k}(z)
$$

and $x_{k}<z_{0}<x_{k+1}$, then what is the value of $s^{\prime \prime \prime}\left(z_{0}\right)$ ? You may assume that $\alpha(0: n+1)$ is given and that $k$ (also given) satisfies $1 \leq k \leq n-1$.

From the local support properties of the basis functions

$$
\begin{aligned}
s^{\prime \prime \prime}\left(z_{0}\right) & =\sum_{j=0}^{n+1} \alpha_{j} B_{j}^{\prime \prime \prime}\left(z_{0}\right) \\
& =\alpha_{k-1} B_{k-1}^{\prime \prime \prime}\left(z_{0}\right)+\alpha_{k} B_{k}^{\prime \prime \prime}\left(z_{0}\right)+\alpha_{k+1} B_{k+1}^{\prime \prime \prime}\left(z_{0}\right)+\alpha_{k+2} B_{k+2}^{\prime \prime \prime}\left(z_{0}\right)
\end{aligned}
$$

8 points for recognizing that.
Using the definition of the basis functions and chain rule:
$s^{\prime \prime \prime}\left(z_{0}\right)=\frac{1}{h^{3}}\left(\alpha_{k-1} B_{*}^{\prime \prime \prime}\left(\frac{z_{0}-x_{k-1}}{h}\right)+\alpha_{k} B_{*}^{\prime \prime \prime}\left(\frac{z_{0}-x_{k}}{h}\right)+\alpha_{k+1} B_{*}^{\prime \prime \prime}\left(\frac{z_{0}-x_{k+1}}{h}\right)+\alpha_{k+2} B_{*}^{\prime \prime \prime}\left(\frac{z_{0}-x_{k+2}}{h}\right)\right)$
8 points for that.
Using the given 3 rd derivative facts about $B_{*}$ :

$$
B_{*}^{\prime \prime \prime}\left(\frac{z_{0}-x_{k-1}}{h}\right)=-1 \quad B_{*}^{\prime \prime \prime}\left(\frac{z_{0}-x_{k}}{h}\right)=18 \quad B_{*}^{\prime \prime \prime}\left(\frac{z_{0}-x_{k+1}}{h}\right)=-18 \quad B_{*}^{\prime \prime \prime}\left(\frac{z_{0}-x_{k+2}}{h}\right)=1
$$

9 points for that. Thus, $s^{\prime}\left(z_{0}\right)=\left(-\alpha_{k-1}+18 \alpha_{k}-18 \alpha_{k+1}+\alpha_{k}\right) / h^{3}$.
Minus 5 for $s^{\prime}\left(z_{0}\right)=\left(\alpha_{k-1}-18 \alpha_{k}+18 \alpha_{k+1}-\alpha_{k}\right) / h^{3}$.
5. Recall that Simpson's rule is the 3-point Newton-Cotes rule. Let $S(a, b, n)$ be the composite Simpson rule with $n$ equal subintervals applied to

$$
I(a, b)=\int_{a}^{b} f(x) d x
$$

It can be shown that

$$
|I(a, b)-S(a, b, n)| \leq \frac{M_{4}}{2880 n^{4}}(b-a)^{5}
$$

where $M_{4}$ is an upper bound on the size of $\left|f^{(4)}(x)\right|$.
(a) If the function evaluations associated $S(a, b, 2)$ are available, how many new function evaluations are required to compute $S(a, m, 2)$ where $m=(a+b) / 2$ ? (Drawing a picture is fine.) Why is this fact important when implementing an adaptive Simpson procedure?


5 points for that. Minus 5 if you replace $\mathrm{S}(\mathrm{a}, \mathrm{b}, 2)$ and $\mathrm{S}(\mathrm{a}, \mathrm{m}, 2)$ with $\mathrm{S}(\mathrm{a}, \mathrm{b}, 1)$ and $\mathrm{S}(\mathrm{a}, \mathrm{m}, 1)$ resp.
The re-usable f-evals should be passed through the recursive call to the left half-sized problem. WIll approximately halve the total number of f-evals. 5 points for that.
(b) Suppose the function $f(x)$ satisfies $f(-x)=f(x)$ for all $x$. Outline how the composite Simpson rule can be used to approximate $I(-a, 2 a)$ so that the absolute error is bounded by a given positive tolerance $\delta$. Be sure to explain your strategy for minimizing the total number of $f$-evaluations. (It does not have to be perfect.)

$$
I(-a, 2 a)=2 I(0, a)+I(a, 2 a) \approx 2 S\left(0, a, n_{1}\right)+S\left(a, 2 a, n_{2}\right)
$$

5 points for that
Error requirement:

$$
2 \frac{M_{4}}{2880 n_{1}^{4}} a^{5}+\frac{M_{4}}{2880 n_{2}^{4}} a^{5} \leq \delta
$$

i.e.,

$$
\begin{equation*}
\frac{2}{n_{1}^{4}}+\frac{1}{n_{2}^{4}} \leq \frac{\delta}{2880 M_{4} a^{5}} \equiv \tilde{\delta} \tag{1}
\end{equation*}
$$

5 points for that.
Choosing $n_{1}$ and $n_{2}$. Simple idea. Choose $n_{1}$ so

$$
\frac{2}{n_{1}^{4}} \leq \frac{1}{2} \tilde{\delta}
$$

and hoose $n_{1}$ so

$$
\frac{1}{n_{2}^{4}} \leq \frac{1}{2} \tilde{\delta}
$$

for then (1) is satisfied. 5 points for any idea that works and addresses the idea that we want to minimize $n_{1}+n_{2}$ since the total number of $f$-evals is about $2 n_{1}+1+2 n_{2}+1$.

