Assignment 3

5 June 2020

MAM2046W 2NA KDSMIL001

1. **Deriving a second derivative approximation formula**
   We are looking for an equation that approximates the second derivative and is of the form

$$f''(x) = \lambda_1 f(x) + \lambda_2 f(x+h) + \lambda_3 f(x-h) + \lambda_4 f(x+2h) + \lambda_5 f(x-2h) \tag{1}$$

We can start by finding the Taylor expansions of each function

$$\begin{aligned}
f(x) &= f(x) \\
f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) + \mathcal{O}(h^5) \\
f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) - \mathcal{O}(h^5) \\
f(x+2h) &= f(x) + 2hf'(x) + 2hf''(x) + \frac{8h^3}{3!}f'''(x) + \frac{16h^4}{4!}f^{(4)}(x) + \mathcal{O}(h^5) \\
f(x-2h) &= f(x) - 2hf'(x) + 2hf''(x) - \frac{8h^3}{3!}f'''(x) + \frac{16h^4}{4!}f^{(4)}(x) - \mathcal{O}(h^5)
\end{aligned}$$

and then, after collecting coefficients of derivatives of f, Equation 1 looks like this, ignoring the error term

$$\begin{aligned}
f''(x) = (\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5)f(x) + (\lambda_2 - \lambda_3 + 2\lambda_4 - 2\lambda_5)hf'(x) \\
+(\lambda_2 + \lambda_3 + 4\lambda_4 + 4\lambda_5)h^2 f''(x) + (\lambda_2 - \lambda_3 + 8\lambda_4 - 8\lambda_5)h^3 f'''(x) \\
+(\lambda_2 + \lambda_3 + 16\lambda_4 + 16\lambda_5)h^4 f^{(4)}(x)
\end{aligned} \tag{2}$$

Now we can equate coefficients of derivatives on either side of the equation, which we can turn into a matrix equation:

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & -1 & 2 & -2 \\ 0 & 1 & 1 & 4 & 4 \\ 0 & 1 & -1 & 8 & -8 \\ 0 & 1 & 1 & 16 & 16 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \\ \lambda_5 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \frac{2}{h^2} \\ 0 \\ 0 \end{pmatrix}$$

Solving this equation (finding the inverse of the 5×5 matrix) gives us values for our λ's, which are:

$$\lambda_1 = \frac{-30}{12h^2};\ \ \lambda_2 = \frac{16}{12h^2};\ \ \lambda_3 = \frac{16}{12h^2};\ \ \lambda_4 = \frac{-1}{12h^2};\ \ \lambda_5 = \frac{-1}{12h^2}$$

Finally, we have Equation 1 becoming

$$\begin{aligned} f''(x) &= \frac{-30f(x) + 16f(x+h) + 16f(x-h) - f(x+2h) - f(x-2h)}{12h^2} \\ &= \frac{-f(x-2h) + 16f(x-h) - 30f(x) + 16f(x+h) - f(x+2h)}{12h^2} \end{aligned} \tag{3}$$

2. **Evaluating an integral with the Composite Trapezoid Method**
   We aim to evaluate the following integral using the composite trapezoid method, using n equal subintervals

$$I = \int_a^b e^x dx \tag{4}$$

Firstly, we can look at the general form of the trapezoid method for approximating an integral:

$$\int_a^b f(x)dx = \underbrace{\frac{h}{2}\sum_{i=0}^{n-1}[f(x_i) + f(x_{i+1})]}_{\text{approximation}} - \underbrace{\frac{h^2}{12}(b-a)f''(c)}_{\text{error}} \tag{5}$$

where n is the number of equal subintervals between a and b, $h = (a-b)/n$, and $c \in [a, b]$. c is arbitrary but we choose it to be the point which maximises $f''(x)$ on the given interval in order to look at the "worst case scenario", if you will. Applying Equation 5 to Equation 4, and ignoring the error term for now, we get

$$\begin{aligned} I &\approx \frac{h}{2}\sum_{i=0}^{n-1}[e^{x_i} + e^{x_{i+1}}] \\ &= \frac{h}{2}\left[\sum_{i=0}^{n-1} e^{x_i} + \sum_{i=0}^{n-1} e^{x_{i+1}}\right] \end{aligned}$$

These sums can be converted into 2 geometric series as each has a common ratio of e^h, therefore we get

$$I \approx \frac{h(1-e^{hn})}{2(1-e^h)}[e^a + e^{a+h}] \tag{6}$$

Of course, this is only an approximation as we haven't included the error term yet. In this error term though, there is $f''(c)$, where c is the the point which maximises f''. In this case, $c = b$ as $f''(x) = e^x$ is strictly increasing everywhere. So finally we have

$$I = \frac{h(1-e^{hn})}{2(1-e^h)}[e^a + e^{a+h}] - \frac{h^2}{12}(b-a)f''(b) \tag{7}$$

3. **Implementing the Composite Midpoint Method**
   The composite midpoint method has the general form of

$$\int_a^b f(x)dx = \underbrace{h\sum_{i=0}^{n-1} f(w_i)}_{\text{approximation}} + \underbrace{\frac{h^2(b-a)}{24}f''(c)}_{\text{error}} \tag{8}$$

where $h = (b-a)/n$, $w_i = a + (i + \frac{1}{2})h$, and $c \in [a, b]$. Again, we choose c to be the value which maximises f'', to get a worst case scenario for the error. We were to use this method to estimate

$$\int_0^1 \frac{4}{1+x^2}dx = \pi \tag{9}$$

with $n = 1000$. Below is our implementation of Equation 8 applied to Equation 9 in Python.

```python
import numpy as np
# Setting constants to allow for modification if need be
a = 0
b = 1
n = 1000
h = (b-a)/n
I = 0
# Looping through the summation, setting a new w at each iteration
for i in range(1000):
    w = a+((i+(1/2))*h)
    I += 4/(1+(w**2))
# Multiplying by h as per the formula
I *= h
print(I)
```

Composite Midpoint Method

When we compute the value of the error term, using $c = 1$ as that maximises the f'', we get a value of $\pi = 3.1415928202531225$. The difference between this and the known value of π is $\approx 1.667 \times 10^{-7}$. This is quite good.