Numerical Analysis Assignment 3

CNNAUA001

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Analytical Problems

1. Derive the following second derivative approximation formula

$$f''(x) = \frac{-f(x+2h) + 16f(x+h) - 30f(x) + 16f(x-h) - f(x-2h)}{12h^2} \tag{1}$$

You may neglect the error term

In order to find equation (1), I will take the Taylor Expansion of $f(x), f(x+h), f(x-h), f(x+2h)$ and $f(x-2h)$:

$$\begin{aligned}
f(x) &= f(x) \\
f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(x) + O(h^5) \\
f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(x) + O(h^5) \\
f(x+2h) &= f(x) + 2hf'(x) + \frac{4h^2}{2}f''(x) + \frac{8h^3}{6}f'''(x) + \frac{16h^4}{24}f^{(4)}(x) + O(h^5) \\
f(x-2h) &= f(x) - 2hf'(x) + \frac{4h^2}{2}f''(x) - \frac{8h^3}{6}f'''(x) + \frac{16h^4}{24}f^{(4)}(x) + O(h^5)
\end{aligned}$$

Now to find the coefficients, and neglecting the higher orders:

$$\begin{aligned}
af(x) &= af(x) \\
bf(x+h) &= bf(x) + bhf'(x) + b\frac{h^2}{2}f''(x) + b\frac{h^3}{6}f'''(x) + b\frac{h^4}{24}f^{(4)}(x) \\
cf(x-h) &= cf(x) - chf'(x) + c\frac{h^2}{2}f''(x) - c\frac{h^3}{6}f'''(x) + c\frac{h^4}{24}f^{(4)}(x) \\
df(x+2h) &= df(x) + d2hf'(x) + d\frac{4h^2}{2}f''(x) + d\frac{8h^3}{6}f'''(x) + d\frac{16h^4}{24}f^{(4)}(x) \\
ef(x-2h) &= ef(x) - e2hf'(x) + e\frac{4h^2}{2}f''(x) - e\frac{8h^3}{6}f'''(x) + e\frac{16h^4}{24}f^{(4)}(x)
\end{aligned}$$

Adding the equations gives:

$$\begin{aligned}
af(x)+bf(x+h)+cf(x-h)+df(x+2h)+ef(x-2h) &= bhf'(x)+b\frac{h^2}{2}f''(x)+ \\
b\frac{h^3}{6}f'''(x) + b\frac{h^4}{24}f^{(4)}(x) &+ cf(x) - chf'(x) + c\frac{h^2}{2}f''(x) \\
- c\frac{h^3}{6}f'''(x) + c\frac{h^4}{24}f^{(4)}(x) &+ df(x) + d2hf'(x) + d\frac{4h^2}{2}f''(x)
\end{aligned}$$

$$+d\frac{8h^3}{6}f'''(x)+d\frac{16h^4}{24}f^{(4)}(x)+ef(x)-e2hf'(x)+e\frac{4h^2}{2}f''(x)-e\frac{8h^3}{6}f'''(x)+e\frac{16h^4}{24}f^{(4)}(x)$$

$$\therefore af(x)+bf(x+h)+cf(x-h)+df(x+2h)+ef(x-2h) = (a+b+c+d+e)f(x)+(b-c+2d-2e)hf'(x)$$

$$+(b+c+4d+4e)\frac{h^2}{2}f''(x)+(b-c+8d-8e)\frac{h^3}{6}f'''(x)+(b+c+16d+16e)\frac{h^4}{24}f^{(4)}$$

And from equation (1) we see that we want this in terms of $f''(x)$ only, therefore we set the others to zero as follows:

$$\begin{aligned}
(a+b+c+d+e) &= 0 \\
(b-c+2d-2e) &= 0 \\
(b+c+4d+4e) &= 1 \\
(b-c+8d-8e) &= 0 \\
(b+c+16d+16e) &= 0
\end{aligned}$$

This can be written as an augmented matrix:

$$\left[\begin{array}{ccccc|c}
1 & 1 & 1 & 1 & 1 & 0 \\
0 & 1 & -1 & 2 & -2 & 0 \\
0 & 1 & 1 & 4 & 4 & 1 \\
0 & 1 & -1 & 8 & -8 & 0 \\
0 & 1 & 1 & 16 & 16 & 0
\end{array}\right]$$

$$\left[\begin{array}{ccccc|c} 1 & 0 & 2 & -1 & 3 & 0 \\ 0 & 1 & -1 & 2 & -2 & 0 \\ 0 & 0 & 2 & 2 & 6 & 1 \\ 0 & 0 & 0 & 6 & -6 & 0 \\ 0 & 0 & 2 & 14 & 18 & 0 \end{array}\right]$$

$$\left[\begin{array}{ccccc|c} 1 & 0 & 0 & -3 & -3 & -1 \\ 0 & 1 & 0 & 3 & 1 & \frac{1}{2} \\ 0 & 0 & 1 & 1 & 3 & \frac{1}{2} \\ 0 & 0 & 0 & 6 & -6 & 0 \\ 0 & 0 & 0 & 12 & 12 & -1 \end{array}\right]$$

$$\left[\begin{array}{ccccc|c} 1 & 0 & 0 & -3 & -3 & -1 \\ 0 & 1 & 0 & 3 & 1 & \frac{1}{2} \\ 0 & 0 & 1 & 1 & 3 & \frac{1}{2} \\ 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 1 & 1 & -\frac{1}{12} \end{array}\right]$$

$$\left[\begin{array}{ccccc|c} 1 & 0 & 0 & -3 & -3 & -1 \\ 0 & 1 & 0 & 3 & 1 & \frac{1}{2} \\ 0 & 0 & 1 & 1 & 3 & \frac{1}{2} \\ 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -\frac{1}{24} \end{array}\right]$$

$$\left[\begin{array}{ccccc|c} 1 & 0 & 0 & -3 & -3 & -1 \\ 0 & 1 & 0 & 3 & 1 & \frac{1}{2} \\ 0 & 0 & 1 & 1 & 3 & \frac{1}{2} \\ 0 & 0 & 0 & 1 & 0 & -\frac{1}{24} \\ 0 & 0 & 0 & 0 & 1 & -\frac{1}{24} \end{array}\right]$$

$$\left[\begin{array}{ccccc|c} 1 & 0 & 0 & 0 & 0 & -\frac{5}{4} \\ 0 & 1 & 0 & 0 & 0 & \frac{2}{3} \\ 0 & 0 & 1 & 0 & 0 & \frac{2}{3} \\ 0 & 0 & 0 & 1 & 0 & -\frac{1}{24} \\ 0 & 0 & 0 & 0 & 1 & -\frac{1}{24} \end{array}\right]$$

It is now seen that:

$$a = -\frac{5}{4}$$
$$b = \frac{2}{3}$$
$$c = \frac{2}{3}$$
$$d = -\frac{1}{24}$$
$$e = -\frac{1}{24}$$

Now substituting these back into the equation:

$$af(x)+bf(x+h)+cf(x-h)+df(x+2h)+ef(x-2h) = (a+b+c+d+e)f(x)+(b-c+2d-2e)hf'(x)$$
$$+(b+c+4d+4e)\frac{h^2}{2}f''(x)+(b-c+8d-8e)\frac{h^3}{6}f'''(x)+(b+c+16d+16e)\frac{h^4}{24}f^{(4)}$$

to get:

$$-\frac{5}{4}f(x)+\frac{2}{3}f(x+h)+\frac{2}{3}f(x-h)-\frac{1}{24}f(x+2h)-\frac{1}{24}f(x-2h)=\frac{h^2}{2}f''(x)$$
$$\therefore -\frac{5}{2}f(x)+\frac{4}{3}f(x+h)+\frac{4}{3}f(x-h)-\frac{1}{12}f(x+2h)-\frac{1}{12}f(x-2h)=h^2f''(x)$$
$$\therefore f''(x)=\frac{-30f(x)+16f(x+h)+16f(x-h)-f(x+2h)-f(x-2h)}{12h^2} \tag{2}$$

With some rearrangement of the numerator this becomes:

$$f''(x)=\frac{-f(x+2h)+16f(x+h)-30f(x)+16f(x-h)-f(x-2h)}{12h^2}$$

Which is the same as equation (1).

2. Use the composite Trapezoid method to evaluate the integral

$$I=\int_a^b e^x dx \tag{3}$$

using n equal subintervals. Your answer should be in closed form and should not include the summation symbol.

Writing equation (3) in the way defined by the Trapezoid method we get:

$$\int_a^b e^x dx=\frac{h}{2}\sum_{i=0}^{n-1}[f(x_i)+f(x_{i+1})]-\frac{h^3}{12}\sum_{i=0}^{n-1}f''(\zeta_i)$$
$$\therefore \int_a^b e^x dx=\frac{h}{2}\sum_{i=0}^{n-1}[f(x_i)+f(x_{i+1})]-\frac{h^3}{12}nf''(c)$$

For the function e^x, as it is a growing exponential, the maximum will occur at e^b, which means that $f''(c)=e^b$. The equation becomes:

$$\therefore \int_a^b e^x dx=\frac{h}{2}\sum_{i=0}^{n-1}[f(x_i)+f(x_{i+1})]-\frac{h^2(b-a)}{12}e^b$$
$$\therefore \int_a^b e^x dx=\frac{h}{2}\Big(\sum_{i=0}^{n-1}f(x_i)+\sum_{i=0}^{n-1}f(x_{i+1})\Big)-\frac{h^2(b-a)}{12}e^b$$

Focusing on the summation part, using the expression for the sum of a geometric series, we can rewrite the summation.
For $\sum_{i=0}^{n-1} f(x_i)$:

$$\sum_{i=0}^{n-1} f(x_i) = \sum_{i=0}^{n-1} e^{x_i}$$

Applying the sum of a geometric series formula:

$$S_n = \frac{a(1-r^n)}{1-r}$$

Where a is the first term, r is the common ratio, and n is the number of terms.

$$\begin{aligned} a &= e^{x_i} = e^a \\ r &= \frac{e^{x_i+1}}{e^{x_i}} = e^{x_{i+1}-x_i} \\ n &= \frac{b-a}{h} \end{aligned}$$

Aside, we know that each value is incremented by h which means that $x_i + h = x_{i+1} \implies h = x_{i+1} - x_i$

$$\therefore r = e^h$$

Now substituting these values into the expression:

$$\begin{aligned} S_n &= \frac{e^a\Big(1-(e^h)^n\Big)}{1-e^h} \\ \therefore S_n &= \frac{e^a\Big(1-(e^h)^{(\frac{b-a}{h})}\Big)}{1-e^h} \\ \therefore S_n &= \frac{e^a - e^a(e^{b-a})}{1-e^h} \\ \therefore S_n &= \frac{e^a - e^b}{1-e^h} \end{aligned}$$

For $\sum_{i=0}^{n-1} f(x_i)$:
Now:

$$\begin{aligned} a &= e^{x_{i+1}} = e^{a+h} \\ r &= \frac{e^{x_{i+2}}}{e^{x_{i+1}}} = e^h \\ n &= \frac{b-a}{h} \end{aligned}$$

The expression is then:

$$S_n = \frac{e^{a+h}\Big(1-(e^h)^n\Big)}{1-e^h}$$
$$\therefore S_n = \frac{e^{a+h}\Big(1-(e^h)^{(\frac{b-a}{h})}\Big)}{1-e^h}$$
$$\therefore S_n = \frac{e^{a+h}-e^{a+h}(e^{b-a})}{1-e^h}$$
$$\therefore S_n = \frac{e^a e^h - e^b e^h}{1-e^h}$$
$$\therefore S_n = \frac{e^h(e^a-e^b)}{1-e^h}$$

Now putting these together gives the full summation:

$$\sum_{i=0}^{n-1}[f(x_i)+f(x_{i+1})] = \frac{e^a-e^b}{1-e^h} + \frac{e^h(e^a-e^b)}{1-e^h}$$
$$\therefore \sum_{i=0}^{n-1}[f(x_i)+f(x_{i+1})] = \frac{(e^a-e^b)(1+e^h)}{1-e^h}$$
$$\therefore \sum_{i=0}^{n-1}[f(x_i)+f(x_{i+1})] = \frac{(e^h+1)(e^a-e^b)}{1-e^h}$$

Now putting this into the Trapezoid method:

$$\int_a^b e^x dx = \frac{h}{2}\Big(\frac{(e^h+1)(e^a-e^b)}{1-e^h}\Big) - \frac{h^2(b-a)}{12}e^b$$

Therefore the evaluated integral is $I = \frac{h}{2}\Big(\frac{(e^h+1)(e^b-e^a)}{e^h-1}\Big)$ with the error term being $-\frac{h^2(b-a)}{12}e^b$.

Numerical Problems

3. Use the Composite Midpoint method with $n = 1000$ to estimate the integral

$$\int_0^1 \frac{4}{1+x^2}dx = \pi \qquad (4)$$

For the numerical part I created the function:

$$f(x) = \frac{4}{1+x^2}$$

and found it's first and second derivative, as that is what we need for the composite midpoint method, which is:

$$f'(x) = -\frac{8x}{(1+x^2)^2}$$
$$f''(x) = -\frac{8(-3x^2+1)}{(1+x^2)^3}$$

In order to find a critical point of the graph, I set $f'(x)$ to zero:

$$f'(x) = -\frac{8x}{(1+x^2)^2} = 0$$
$$\therefore 8x = 0$$
$$\therefore x = 0$$

So at $x = 0$ there is a critical point, and if we plug this into the second derivative we get:

$$f''(0) = -\frac{8(-3(0)^2+1)}{(1+(0)^2)^3}$$
$$\therefore f''(0) = -8$$

This means that at this point the graph is concave down, and if we look at the graph in Figure (1) we see that at $x = 0$, the graph is concave down and we have a maximum.

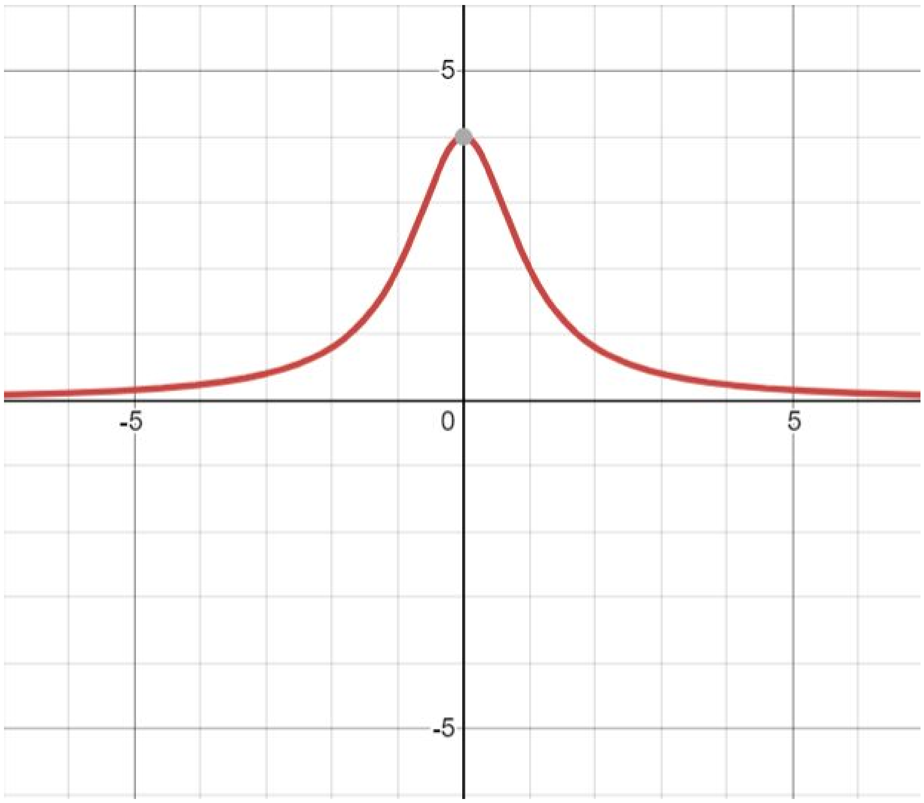

Figure 1: A graph of $f(x)$

Now that we have this information, we can begin using the method. In my code I defined $f(x)$ and $f''(x)$ as well as the midpoint as w which takes in an increment, a starting value and the step and outputs the midpoint between the two values. This is seen in the code in the appendix. All of this is then used in the Composite Midpoint Method where I add all of the areas of the rectangles into an array called "area" and then find the total area by summing all of the values in the array as well as adding the error term to them. In this case it is:

$$\frac{h^2}{24}f''(c) = \frac{h^2}{24}f''(0) = -\frac{h^2}{3}$$

The code then prints out the value of the area as well as the actual value of π and the absolute error, to see how accurate this method and function was at determining π. It is seen that the value obtained from the code is:

$$\pi_{code} = 3.141592403589793$$
$$\pi = 3.141592653589793$$
$$\therefore |\pi - \pi_{code}| = 2.500000002569891 \times 10^{-7}$$

Therefore it is seen that this is a good approximation of pi as it has a very small absolute error and it is seen as the approximation is the same as pi up to six decimal places.

Appendix

Code for Question 3

```
# Question 3 of NA
# CNNAUA001
# 10/6/2020

## Importing Libraries ---------------------------------------------------------
import numpy as np
import scipy as sc
import matplotlib.pyplot  as plt
from matplotlib import rc
##------------------------------------------------------------------------------

## Initialising Variables & Arrays ---------------------------------------------
n = 1000
a = 0                                       # Intitial value
b = 1                                       # Final value
h = (b - a) / n                             # Increment
i = 0                                       # Index
area = []                                   # Array that stores area
##------------------------------------------------------------------------------

## Defining the Functions ------------------------------------------------------
def f(x):
    y = 4 / (1+x**2)
    return y

def fdp(x):                                 # Second derivative of f(x)
    y = -((8*(-3*x**2+1))/(1+x**2)**3)
    return y

def w(i,a,h):                               # Midpoint function
    y = a + (i + 0.5)*h
    return y
##------------------------------------------------------------------------------

## Composite Midpoint method ---------------------------------------------------
while i < n:
    area.append(h*f(w(i,a,h)))              # Stores rectangle areas
    i += 1
Area = np.sum(area) + (h**2 / 24)*(fdp(0))  # Finds the total area
##------------------------------------------------------------------------------

## Printing --------------------------------------------------------------------
```

```
print('Estimate of pi is: ',Area)
print('pi is actually: ',np.pi)
print('Absolute error is:', abs(np.pi - Area))
##--------------------------------------------------------------------------------
```

The output is:

```
Estimate of pi is:  3.141592403589793
pi is actually:  3.141592653589793
Absolute error is: 2.500000002569891e-07
```