CALIFORNIA INSITUTE OF TECHNOLOGY

Ph20 Assignment 3

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1 QUESTION 1

Simpson's formula for integrating $f(x)$ between points $x = a$ and $x = b$ is :

$$\int_a^b f(x)dx = H\left(\frac{f(a)}{6} + \frac{4f(c)}{6} + \frac{f(b)}{6}\right) \tag{1.1}$$

where $c = \frac{b-a}{2}$. Using Taylor's expansions series to an order up to 4, we can evaluate the error of the approximation.

$$f(b) = f(a) + f'(a)H + \frac{f''(a)}{2!}H^2 + \frac{f'''(a)}{3!}H^3 + \frac{f''''(\eta)}{4!}H^4 \tag{1.2}$$

$$f(c) = f(a) + f'(a)\frac{H}{2} + \frac{f''(a)}{2!}\left(\frac{H}{2}\right)^2 + \frac{f'''(a)}{3!}\left(\frac{H}{2}\right)^3 + \frac{f''''(\eta)}{4!}\left(\frac{H}{2}\right)^4 \tag{1.3}$$

where η is the Lagrangian remainder. Using the top integral (1.1) the estimated integral is:

$$I_{simp} = H\left(f(a) + \frac{f'(a)}{2}H + \frac{f''(a)}{6}H^2 + \frac{f'''(a)}{24}H^3 + \frac{5f''''(\eta)}{576}H^4\right) \tag{1.4}$$

Using taylor expansion for the integral:

$$I = H\left(f(a) + \frac{f'(a)}{2}H + \frac{f''(a)}{6}H^2 + \frac{f'''(a)}{24}H^3 + \frac{f''''(\eta)}{120}H^4\right) \tag{1.5}$$

Calculating the difference between exact and approximation gives an error of order 5 as expected.

$$error_{loc} = I_{simp} - I = \frac{f''''(\eta)}{2880}H^5 \tag{1.6}$$

To show that its global error is of order 4, we need to split Simpson's formula as folllows:

$$\int_a^b f(x)dx = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + ... \int_{x_{2N-2}}^{x_2N} f(x)dx \tag{1.7}$$

Applying Simpson's formula to each part of the integral:

$$I_{simp} = h_N\left(\frac{f(x_0)}{6} + \frac{4f(x_1)}{6} + \frac{f(x_2)}{6}\right) + ...h_N\left(\frac{f(x_{2N-2})}{6} + \frac{4f(x_{2N-1})}{6} + \frac{f(x_2N)}{6}\right) \tag{1.8}$$

which can be re-written as

$$I_{simp} = h_N\left(\frac{f(x_0)}{6} + \frac{f(x_N)}{6} + \frac{2}{3}\sum_{i=0}^{N-1} f(x_{2i+1}) + \frac{1}{3}\sum_{i=1}^{N-1} f(x_{2j})\right) \tag{1.9}$$

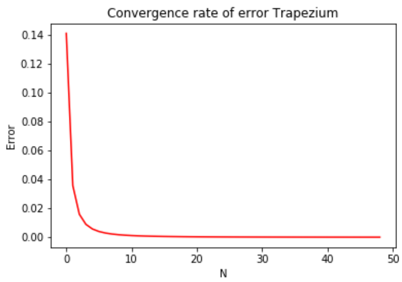
The global error will therefore be N times Equation (1.6) where the width is just h_N

$$error_{glob} = \frac{f''''(\eta)}{2880}h_N^5 N = \frac{f''''(\eta)}{2880}h_N^5\frac{H}{h_N} = H\frac{f''''(\eta)}{2880}h_N^4 \tag{1.10}$$

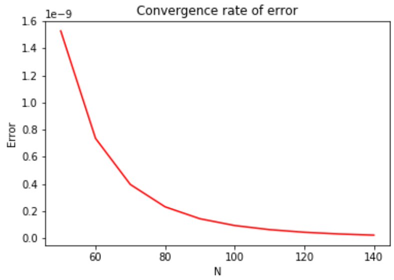
Which is of fourth order as expected.

2 QUESTION 4

Both methods, Trapezium and Simpson's rule converge to the true value of the integral at large values of N. Looking at the two figures below with N =50, and focusing on the error axis, the Simpson's rule seems to converge to the correct value much faster than the trapezium rule. This shows that the Simpson's rule is more accurate.



(a) Trapezium Rule N=50



(b) Simpson's Rule N=50

3 QUESTION 5

Both Trapezium rule and Simpson's rule follow the expected pattern. There is a relatively large uncertainty in the first values of N (N ~ 10), but there is an exponential decay as the value of N grows larger. For very large values of N (N ~ 1000) a small deviation starts to appear which seems to make the error fluctuate.

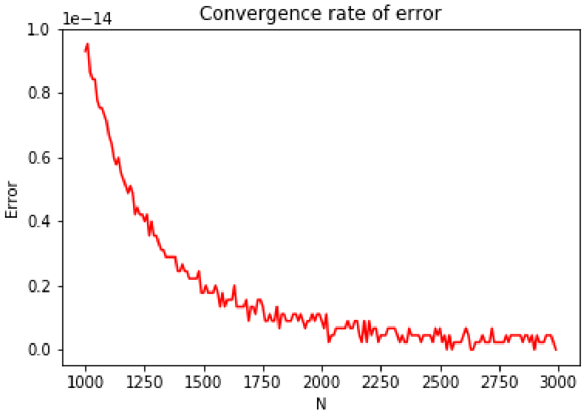


Figure 3.1: Simpson's Rule N=1000

4 Question 7

Comparing results of scipy.integrate.quad and scipy.integrate.romberg with the trapezium rule and simpson's rule they seem to converge both faster and the error is way less. Looking at program Ph20_A3_ 3.py it can easily be seen that the difference in the error between the manual methods and the ready - made functions of scipy are in the order of $\sim 10^{-12}$.

This shows that these methods for integrating are a lot more effective than the approximations we used in this assignment.