Ph20: Assignment 2

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1 Extended Simpson's Formula

Let $I = \int_a^b f(x)\ dx$ and $h_N = (b-a)/N$, where $x_0 = a, x_1 = a + h_N, x_2 = a + 2h_N, \dots, x_N = b$. Since

$$I_{\text{simp}} = H\left(\frac{f(a)}{6} + \frac{4f(c)}{6} + \frac{f(b)}{6}\right),$$

where $H = b - a$ and $c = (a+b)/2$, then the extended Simpson's Formula is:

$$\begin{aligned}
\int_a^b f(x)\ dx &= \int_{x_0}^{x_1} f(x)\ dx + \int_{x_1}^{x_2} f(x) + \cdots \int_{x_{N-1}}^{x_N} f(x)\ dx \\
&\simeq h_N\left(\frac{f(x_0)}{6} + \frac{4f(\frac{x_0+x_1}{2})}{6} + \frac{f(x_1)}{6}\right) + h_N\left(\frac{f(x_1)}{6} + \frac{4f(\frac{x_1+x_2}{2})}{6} + \frac{f(x_2)}{6}\right) \\
&\qquad + \cdots + h_N\left(\frac{f(x_{N-1})}{6} + \frac{4f(\frac{x_{N-1}+x_N}{2})}{6} + \frac{f(x_N)}{6}\right) \\
&= \frac{h_N}{6}\Bigg\{ f(x_0) + f(x_N) + 2[f(x_1) + f(x_2) + \cdots + f(x_{N-1})] \\
&\qquad + 4\left[f\left(\frac{x_0+x_1}{2}\right) + f\left(\frac{x_1+x_2}{2}\right) + \cdots + f\left(\frac{x_{N-1}+x_N}{2}\right)\right]\Bigg\}
\end{aligned}$$

1.1 Local and Global Error

The Taylor expansion for $x \in [a,b]$ centered at a is

$$f(x) = f(a) + f'(a)(x-a) + f^{(2)}(a)\frac{(x-a)^2}{2!} + f^{(3)}(a)\frac{(x-a)^3}{3!} + f^{(4)}(\eta)\frac{(x-a)^4}{4!} \qquad \text{with } \eta \in [a,b].$$

Integrating this we get

$$I = f(a)H + f'(a)\frac{H^2}{2!} + f^{(2)}(a)\frac{H^3}{3!} + f^{(3)}(a)\frac{H^2}{4!} + f^{(4)}(\eta)\frac{H^5}{5!} \qquad \text{with } \eta \in [a,b].$$

Using (1.1) to approximate $f(b)$ and $f(c)$,

$$f(b) \simeq f(a) + f'(a)H + f^{(2)}(a)\frac{H^2}{2!} + f^{(3)}(a)\frac{H^3}{3!} + f^{(4)}(\eta)\frac{H^4}{4!}$$
$$f(c) \simeq f\left(\frac{a+b}{2}\right) = f(a) + f'(a)\frac{H}{2} + f^{(2)}(a)\frac{H^2}{8} + f^{(3)}(a)\frac{H^3}{48} + f^{(4)}(\eta)\frac{H^4}{384}.$$

Then $I_{\text{simp}} = H\left[f(a) + f'(a)\frac{H}{2} + f^{(2)}(a)\frac{H^2}{6} + f^{(3)}(a)\frac{H^3}{24} + f^{(4)}(\eta)\frac{5H^4}{576}\right]$, with $\eta \in [a,b]$.

The local error is

$$I_{\text{simp}} - I = \frac{5}{576}f^{(4)}(\eta)H^5 - \frac{1}{5!}f^{(4)}(\eta)H^5 = f^{(4)}(\eta)\frac{H^5}{2880}.$$

and the global error is

$$-f^{(4)}(\varepsilon)\frac{h_N^5}{2880} = -(b-a)f^{(4)}(\varepsilon)\frac{h_N^4}{2880} \qquad \text{with } \varepsilon \in [a,b].$$

2 Evaluating the Trapezoidal and Simpson's Formula

We will evaluate the integral of e^x with each of these formulas. Since $\int_0^1 e^x\ dx = e^x - 1$, we have for the errors $E_{\text{trap}}(N)$ and $E_{\text{simp}}(N)$:

$$E_{\text{trap}}(N) = |(e^x - 1) - I_{\text{trap}}(N;\ e^x, 0, 1)|$$

$$E_{\text{simp}}(N) = |(e^x - 1) - I_{\text{simp}}(N;\ e^x, 0, 1)|$$

where $I_{\text{trap}}(N;\ e^x, 0, 1)$ and $I_{\text{simp}}(N;\ e^x, 0, 1)$ represent the integral of e^x over $[0,1]$ evaluated with the trapezoidal and Simpson's formula respectively.

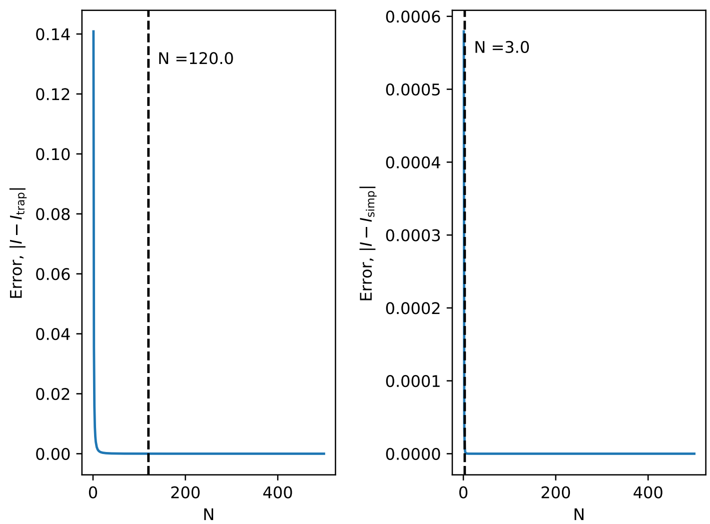

Figure 1: Plot of the errors $E_{\text{trap}}(N)$ and $E_{\text{simp}}(N)$ over $1 \leq N \leq 500$. The dashed line shows the number of partitions N required to obtain an error $\leq 10^{-5}$. Simpson's formula only requires $N = 3$ to achieve this, while the trapezoidal formula requires $N = 120$. This is because the Lagrange polynomial interpolation of the curve underlying Simpson's formula more accurately approximates the shape of the curve.

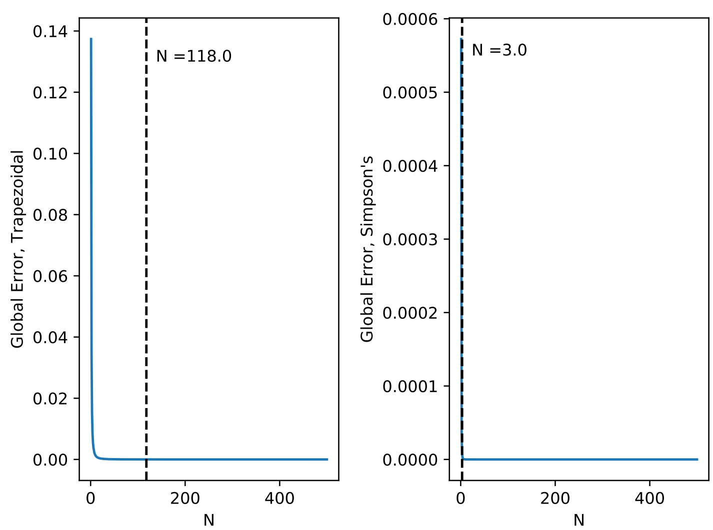

Figure 2: Plot of the predicted global errors for each formula, divided by $f^{(4)}(\varepsilon)$ for $\varepsilon \in [0, 1]$.

Eventually the error plateaus and stops decreasing. This is due to the finite precision of computers in computing numbers with a lot of decimal places.

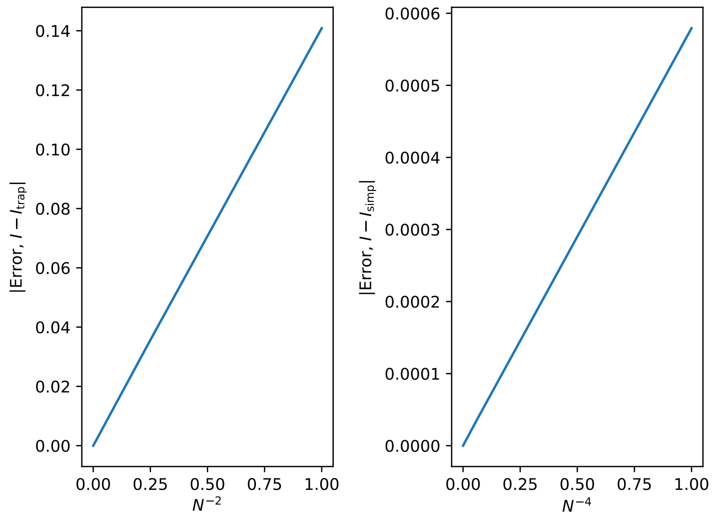

Figure 3: Plot of the errors $E_{\text{trap}}(N)$ and $E_{\text{simp}}(N)$ against N^{-2} and N^{-4} respectively. The linear graphs show that the programs' errors follow the predicted errors' dependence on N.

2.1 Comparing Against `scipy.integrate.quad` and `scipy.integrate.romberg`

Method	Value	Error
Trapazoidal	1.71828197165	$1.43190150181 \times 10^{-7}$
Simpson's	1.71828182846	$6.66133814775 \times 10^{-16}$
`scipy.integrate.quad`	1.7182818284590453	$2.220446049250313 \times 10^{-16}$
`scipy.integrate.romberg`	1.71828182846	$3.30846461338 \times 10^{-14}$

Table 1: Value and errors for $\int_0^1 e^x \, dx$ computed with different methods. The trapezoidal and Simpson's formula were evaluated with $N = 1000$. For this value of N, Simpson's formula gives a smaller error than `romberg` and of same order of magnitude as `quad`. The trapezoidal rule gives an error that is ~ 8 orders of magnitude higher than the rest.

3 Evaluating the General Purpose Routine

The general purpose routine (Question 6) is used to evaluate the integral of e^x over $[0, 1]$ and the integral of $\cos(x)$ over $[0, \pi/4]$.

Function	Relative Accuracy	Iterations	N
e^x	10^{-9}	1	100
	10^{-14}	4	1600
$\cos(x)$	10^{-14}	3	800

Table 2: $\int_0^1 e^x \, dx$ and $\int_0^{(\pi/4)} \cos(x) \, dx$ evaluated with the general routine.

Method	Accuracy	N
Trapezoidal	10^{-9}	11722
Simpson's	10^{-9}	28
	10^{-14}	496

Table 3: The number of partitions N required for the trapezoidal and Simpson's formula to achieve an accuracy of 10^{-9} and 10^{-14} for $\int_0^1 e^x \, dx$. The trapezoidal formula requires ~ 400 times more partitions than Simpson's formula to achieve an accuracy of 10^{-9}. Comparing with Table 2, much higher values of N are required to achieve the same levels of relative accuracy than accuracy alone.