Physics 20 Lab 2

Alexander Zlokapa

October 13, 2017

1 Simpson's Formula

1.1 Derivation of Extended Formula

Similarly to finding the extended trapezoidal formula, we will take Simpson's rule

$$I_{\text{simp}} \equiv H\left(\frac{f(a)}{6} + \frac{4f((a+b)/2)}{6} + \frac{f(b)}{6}\right)$$

where $H = (b-a)$, and apply it to each of N subintervals in the integral:

$$\begin{aligned}
\int_a^b f(x)\,\mathrm{d}x &= \int_{x_0}^{x_1} f(x)\,\mathrm{d}x + \int_{x_1}^{x_2} f(x)\,\mathrm{d}x + \cdots + \int_{x_{N-1}}^{x_N} f(x)\,\mathrm{d}x \\
&\simeq h_N\left(\frac{f(x_0)}{6} + \frac{4f(x_{0.5})}{6} + \frac{f(x_1)}{6}\right) + \cdots + h_N\left(\frac{f(x_{N-1})}{6} + \frac{4f(x_{N-0.5})}{6} + \frac{f(x_N)}{6}\right) \\
&= h_N\left(\frac{f(x_0)}{6} + \frac{1}{3}\sum_{i=1}^{N-1} f(x_i) + \frac{2}{3}\sum_{i=1}^{N-1} f(x_{i+0.5}) + \frac{f(x_N)}{6}\right)
\end{aligned}$$

1.2 Local Error

To derive the local error, we first integrate the Taylor expansion for $f(b)$, observing that $H = b-a$ and $x, \eta \in [a, b]$ to produce the following:

$$\begin{aligned}
f(x) &= f(a) + f'(a)(x-a) + f''(a)\frac{(x-a)^2}{2!} + f'''(a)\frac{(x-a)^3}{3!} + f^{(4)}(a)\frac{(x-a)^4}{4!} + \cdots \\
&= f(a) + f'(a)(x-a) + f''(a)\frac{(x-a)^2}{2!} + f'''(a)\frac{(x-a)^3}{3!} + f^{(4)}(\eta)\frac{(x-a)^4}{4!} \\
I &= f(a)H + f'(a)\frac{H^2}{2!} + f''(a)\frac{H^3}{3!} + f'''(a)\frac{H^4}{4!} + f^{(4)}(\eta)\frac{H^5}{5!}
\end{aligned}$$

Combining Simpson's rule and the Taylor expansion, we have:

$$\begin{aligned}
I_{\text{simp}} &= f(a)\frac{H}{6} + f((a+b)/2)\frac{4H}{6} + f(b)\frac{H}{6} \\
&= f(a)\frac{H}{6} + \left(f(a) + f'(a)\frac{H}{2} + f''(a)\frac{H^2}{4\cdot 2!} + f'''(a)\frac{H^3}{8\cdot 3!} + f^{(4)}(\eta)\frac{H^4}{16\cdot 4!}\right)\frac{4H}{6} \\
&\quad + \left(f(a) + f'(a)\frac{H}{2} + f''(a)\frac{H^2}{2!} + f'''(a)\frac{H^3}{3!} + f^{(4)}(\eta)\frac{H^4}{4!}\right)\frac{H}{6} \\
&= f(a)H + f'(a)\frac{H^2}{2!} + f''(a)\frac{H^3}{3!} + f'''\frac{H^4}{4!} + f^{(4)}(\eta)\frac{5H^5}{576}
\end{aligned}$$

Subtracting I from I_{simp}, we can find the local error:

$$\begin{aligned}
I_{\text{simp}} - I &= f^{(4)}(\eta)H^5\left(\frac{5}{576} - \frac{1}{120}\right) \\
&= f^{(4)}(\eta)\frac{H^5}{2880} \\
&= I_1 + O(H^5)
\end{aligned}$$

Thus, the local error is $O(H^5)$.

1.3 Global Error

To derive the global error, we simply note from the extended Simpson's formula that, for some $\xi \in [a, b]$, we have:

$$-f^{(4)}(\xi)\frac{h_N^5}{2880} \cdot N = -(b-a)f^{(4)}(\xi)\frac{h_N^4}{2880}$$

Thus, the global error is $O(h_N^4)$.

2 Comparing Trapezoidal and Simpson's Methods

We will compare the errors of the two methods by integrating $\int_0^1 e^x \, dx$, which is equal to $e^1 - e^0 = e - 1$. Because an analytic solution is known, we can determine the exact errors of trapezoidal and Simpson's integration methods, resulting in the below log-log plot. As expected from the global

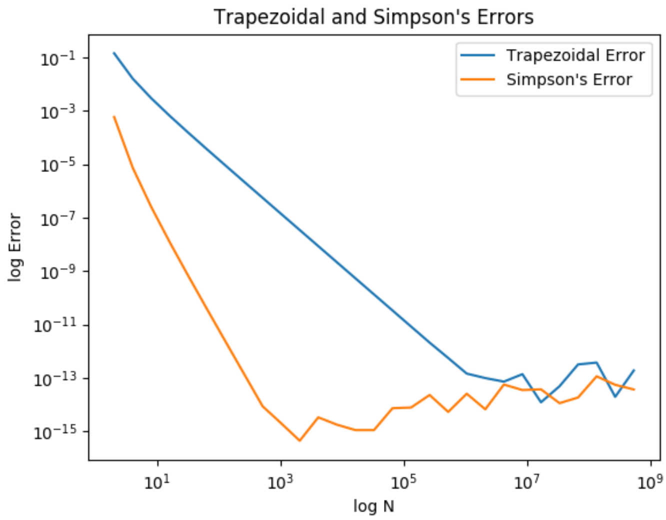

Figure 1: Comparison of errors integrating e^x using trapezoidal integration and Simpson's formula.

errors of the respective methods, the trapezoidal formula results in an error that decreases at the rate of N^{-2}, while Simpson's formula results in an error falloff of N^{-4}. (In other words, increasing the number of subintervals by 2 improves trapezoidal accuracy by a factor of 4 and improves Simpson's accuracy by a factor of 16.) Thus, Simpson's formula proves to converge more quickly to the exact solution.

However, once the error reaches around 10^{-14}, we see a deviation from the expected trend of Simpson's formula's accuracy. This can be explained by floating-point errors caused by the computer's method for storing numbers using a finite number of bits, which makes it impossible to accurately represent an infinite number of decimal places. Indeed, as N increase even further, the floating-point error compounds, worsening the accuracy of the numerical integration methods.

3 Adaptive Simpson's Method

We implemented a general purpose routine for determining an N value sufficiently large to have a relative error below a given bound. Starting with $N_0 = 4$, we increased N_0 by powers of two every iteration. Testing Simpson's method for $\int_0^1 e^x \, dx$ and a relative tolerance of 1E-13, a total of 7 iterations produced a relative error of 8E-14. Testing Simpson's method for $\int_0^\pi \sin x \, dx$ and a relative tolerance of 1E-13, a total of 9 iterations produced a relative error of 6E-14. Thus, our implementation of Simpson's method yielded reasonably accurate results.

4 Other Integration Methods

We integrated e^x from 0 to 1 using trapezoidal, Simpson's, quadrature, and Romberg's methods. The results of all of these were compared to the analytical solution $(e - 1)$, and are summarized below:

- Trapezoidal: 1.7182818284591896
- Simpson: 1.7182818284590706
- Quadrature: 1.7182818284590453
- Romberg: 1.7182818284590782
- Analytical: 1.718281828459045

To twelve decimal places, these methods all yield the same result, although they converge at different rates and thus take different times to compute these results.