Ph20 Lab 2: Intro to Numerical Techniques

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Question 1: Extended Simpson's formula

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

$$\int_a^b f(x)dx = H\left(\frac{f(a)}{6} + \frac{4f(c)}{6} + \frac{f(b)}{6}\right) \tag{1}$$

Where $c = \frac{b-a}{2}$. To evaluate the error, we must consider an approximation up to 4th order in $f(x)$, so we Taylor expand our terms:

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

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

Where η is the Lagrangian remainder. Combining these with Equation 1 we have an estimated integral of:

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

Taylor expanding the exact integral to the same order gives:

$$I = H\left(f(a) + \frac{f'(a)}{2}H + \frac{f''(a)}{6}H^2 + \frac{f'''(a)}{24}H^3 + \frac{f''''(\eta)}{120}H^4\right) \tag{5}$$

The difference between the approximation and exact value gives the error:

$$error_{loc} = I_{simp} - I = \frac{f''''(\eta)}{2880}H^5 \tag{6}$$

Which, as expected, is of order 5 in H.

The extended Simpson formula splits the region [a,b] into N equal sized chunks of size $h_N = \frac{b-a}{N}$. Splitting the integration into these parts too gives:

$$\int_a^b f(x)dx = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + ... \int_{x_{2N-2}}^{x_{2N}} f(x)dx \tag{7}$$

Applying Simpson's formula to each of these chunks:

$$I_{simp} = h_N\left(\frac{f(x_0)}{6} + \frac{4f(x_1)}{6} + \frac{f(x_2)}{6}\right) + h_N\left(\frac{f(x_2)}{6} + \frac{4f(x_3)}{6} + \frac{f(x_4)}{6}\right) + ...h_N\left(\frac{f(x_{2N-2})}{6} + \frac{4f(x_{2N-1})}{6} + \frac{f(x_{2N})}{6}\right) \tag{8}$$

We can rewrite this as:

$$I_{simp} = h_N\left(\frac{f(x_0)}{6} + \frac{f(x_{2N})}{6} + \frac{2}{3}\sum_{i=0}^{N-1} f(x_{2i+1}) + \frac{1}{3}\sum_{i=1}^{N-1} f(x_{2j})\right) \tag{9}$$

As we now have N equal sized chunks, the global error will just be N times the error given by Equation 6, where instead the width is h_N:

$$error_{glob} = \frac{f''''(\eta)}{2880}h_N^5 N = \frac{f''''(\eta)}{2880}h_N^5\frac{H}{h_N} = H\frac{f''''(\eta)}{2880}h_N^4 \tag{10}$$

Which is of fourth order in h_N.

Question 4: Comparing Simpson's and the trapezoidal methods

Figure 1 demonstrates that as the number of steps taken to complete the integration increases, both converge to the true value for $\int_0^1 e^x dx = 1.7182818284590452354$. We see a much faster convergence for Simpson's method, but both clearly approach the correct value. When N is large - for example 10,000 - the Trapezoidal method gives an error of $1 \times 10^{-8}\%$ and the Simpson method an error too small for iPython to handle.

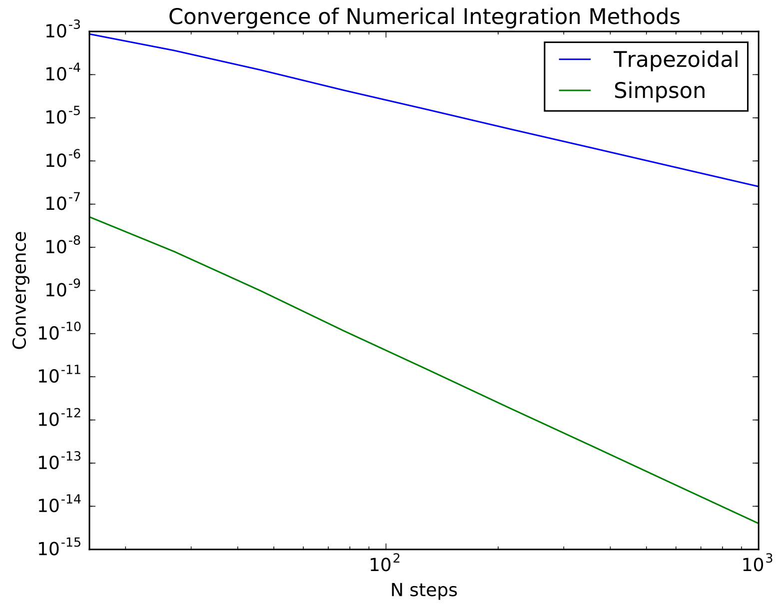

Figure 1: Convergence of the extended Simpson and extended Trapezoidal numerical integration methods to the true value of the integral of e^x from 0 to 1 as the number of steps taken increases.

Question 5: Relative accuracy

The table below shows the number of steps required for the convergence to meet the specified accuracy. Comparison with Figure 1 shows that the function is performing as expected. Convergence occurs at around the same rate for $\cos(x)$

Convergence	e^x	$\cos(x)$
10^{-8}	32	32
10^{-10}	128	128
10^{-12}	512	512
10^{-14}	1024	1024

Question 6: Comparison to scipy

Using scipy.integrate.quad(np.exp, 0, 1) returns an error of the order 1×10^{-12}, a massive improvement on the error obtained using our home-made Trapezoidal method - even at 10,000 steps. It is also signicicantly faster. Using the Romberg method gives an error of the same order, and is also significantly faster.