Computanional Physics - Problem Sheet 1

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1 Derivative Formula

To derive the given 5-point formula for the second derivative of an analytic function $f(x)$, we start from its Taylor expansion around x' to fifth order in $x - x'$

$$f(x) = f(x') + \sum_{n=1}^{5} \frac{(x-x')^n}{n!} f^{(n)}(x') + \mathcal{O}((x-x')^6) \tag{1}$$

For a set of equidistant points x_k with spacing h, implying $x_{k\pm j} - x_k = \pm j \cdot h$, Eq. (1) for $x' = x_k$ yields (we assume that we are far enough away from boundary points)

$$\begin{aligned} f(x_{k\pm j}) =& f(x_k) \pm jhf'(x_k) + \frac{j^2}{2}h^2 f''(x_k) \pm \frac{j^3}{6}h^3 f'''(x_k) \\ &+ \frac{j^4}{24}h^4 f^{(4)}(x_k) \pm \frac{j^5}{120}h^5 f^{(5)}(x_k) + \underbrace{\mathcal{O}((x_{k\pm j} - x_k)^6)}_{\mathcal{O}(h^6)} \end{aligned}$$

Thus,

$$f(x_{k+2}) + f(x_{k-2}) = 2f(x_k) + 4h^2 f''(x_k) + \frac{4}{3}h^4 f^{(4)}(x_k) + \mathcal{O}(h^6)$$

$$f(x_{k+1}) + f(x_{k-1}) = 2f(x_k) + h^2 f''(x_k) + \frac{1}{12}h^4 f^{(4)}(x_k) + \mathcal{O}(h^6)$$

These expressions can be used to remove the fourth order

$$f(x_{k+2}) + f(x_{k-2}) - 16 \cdot (f(x_{k+1}) + f(x_{k-1})) = -30f(x_k) - 12h^2 f''(x_k) + \mathcal{O}(h^6)$$

which can be brought into the desired form using $x_{k\pm j} = x_k \pm jh$

$$f''(x_k) = -\frac{\frac{1}{12}f(x+2h) - \frac{4}{3}f(x+h) + \frac{5}{2}f(x_k) - \frac{4}{3}f(x-h) + \frac{1}{12}f(x-2h)}{h^2} + \mathcal{O}(h^4)$$

2 Simpson Rule

The code for this exercise can be found in the file "cp_ex1_p2.py".

The absolute values of the empirical error together with the upper bound of the theoretical error ($0 \leq f^{(4)}(\zeta) \leq 1$ for $f(x) = \sin(x)$ and $x \in [0, \pi/2]$ thus bounded by $(b-a)h^4/180$) against the width of the slices h can be seen in Fig. 1 where

$$S = \int_0^{\frac{\pi}{2}} \sin(x) = 1 \tag{2}$$

and S_S being the integral approximated by the Simpson rule. The absolute error is plotted to avoid negative values that would not be visible in the logarithmic plot. The lowest possible value for h was limited by the computational resources available.

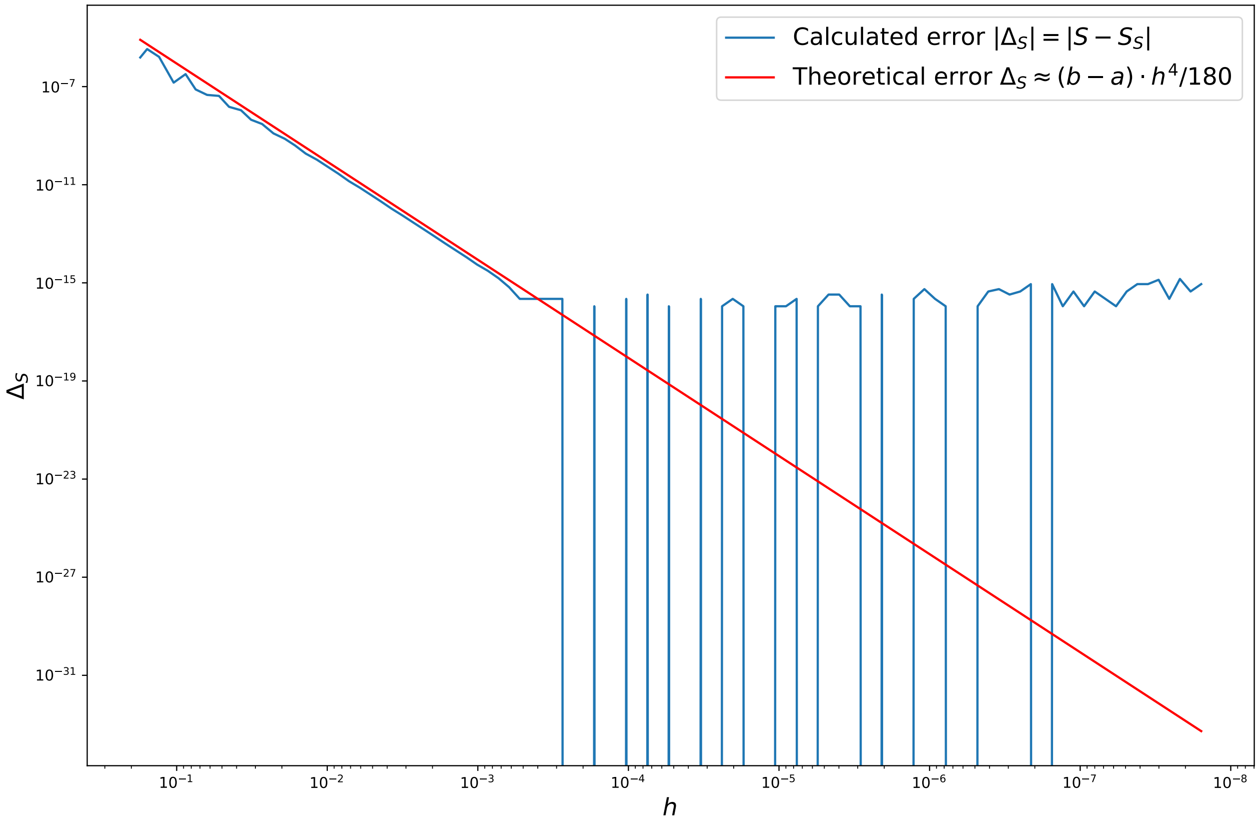

Figure 1: Empirical and theoretical error against point spacing h of the integral S calculated with Simson's rule.

As one can see, the empirical error follows the theoretically predicted h^4 behavior for values of h down to 10^{-4} to 10^{-3} after a small oscillatory period for larger h and is indeed bounded by the theoretical prediction for $f^{(4)}(\zeta) = 1$. The unpredicted behavior for $h < 10^{-4}$ is due to the limited precision of the data type ("double" or "float64", i.e., a 64 bit floating point number) used for the values of the (Simpson and exact) integral. If the difference between exact and numerical value of the integral is smaller than the decimal precision of a "float64" number (which is of order 10^{-16} to 10^{-14}), the error cannot be properly resolved anymore and is either zero or, due to rounding to the last significant digit, is of order of the precision.

3 Romberg Integration

Part 1

To show that the second column of the Neville scheme (denoted as R_{n1}) corresponds to the Simpson rule, we start from the recursion relation of the Romberg integration method

$$R_{nj} = R_{n,j-1} + \frac{1}{4^j - 1}(R_{n,j-1} - R_{n-1,j-1}) \tag{3}$$

for $j = 1$. Since R_{n0} corresponds to the trapezoidal rule with spacing h_n denoted as $S_T(h_n)$, we get

$$R_{n1} = \frac{4}{3} S_T(h_n) - \frac{1}{3} S_T(h_{n-1}) \tag{4}$$

where

$$S_T(h_n) = \frac{h_n}{2} \sum_{k=0}^{2^n-2} (f(x_k) + f(x_{k+1})) \tag{5}$$

and, as shown in the lecture,

$$S_T(h_n) = \frac{1}{2} S_T(h_{n-1}) + h_n \sum_{i=1}^{2^{n-1}} f(x_0 + (2i-1)h_n) \tag{6}$$

Using the previous two equations, we can express Eq. (4) as

$$\begin{aligned}
R_{n1} &= \frac{1}{3}\left(4S_T(h_n) - 2S_T(h_n) + 2h_n \sum_{i=1}^{2^{n-1}} f(x_0 + (2i-1)h_n)\right) \\
&= \frac{h_n}{3}\left(\sum_{k=0}^{2^n-2} (f(x_k) + f(x_{k+1})) + 2\sum_{i=1}^{2^{n-1}} f(x_0 + (2i-1)h_n)\right) \\
&= \frac{h_n}{3}\Big(\underbrace{f(x_0) + 2f(x_1) + 2f(x_2) + ... + 2f(x_{N-3}) + 2f(x_{N-2}) + f(x_{N-1})}_{\text{first sum}} \\
&\quad + \underbrace{2f(x_1) + 2f(x_3) + ... + 2f(x_{N-2})}_{\text{second sum}}\Big)
\end{aligned}$$

where $N = 2^n + 1$ and $x_k = x_0 + k \cdot h_n$. Adding all terms together, we arrive at Simpson's rule S_S for odd numbers of points N

$$R_{n1} = \frac{h_n}{3}\big(f(x_0) + 4f(x_1) + 2f(x_2) + ... + 2f(x_{N-3}) + 4f(x_{N-2}) + f(x_{N-1})\big) \tag{7}$$

$$= S_S \tag{8}$$

Part 2

The code for this exercise can be found in the file "cp_ex1_p3.py".

The results of the Romberg integration method in terms of deviation from the analytic result can be seen in Fig. 2. Here, $S(f(x))$ denotes the analytic result

$$S(f(x)) = \int_a^b f(x)dx$$

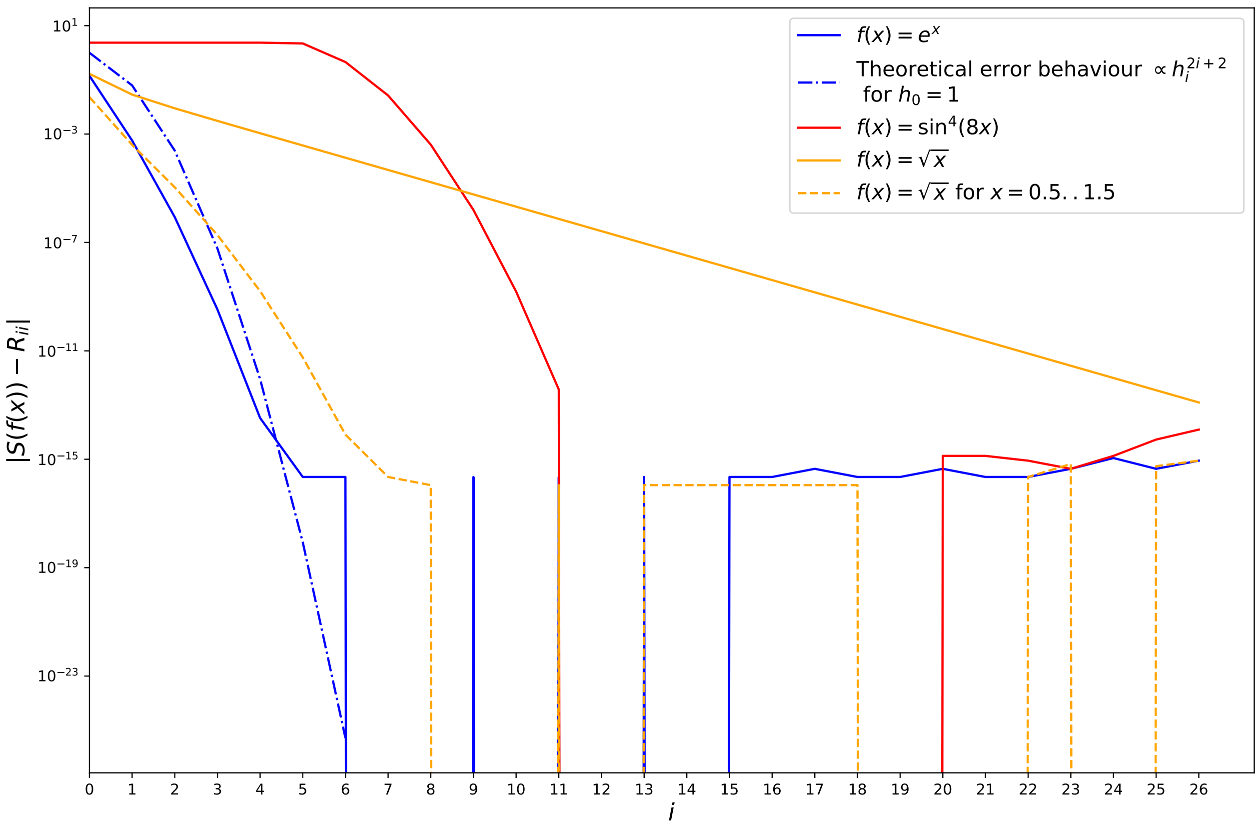

Figure 2: Empirical errors for Romberg integrated functions $f(x)$ using the given integration limits. Also shown are the theoretical error behavior and the result for $f(x) = \sqrt{x}$ with shifted integration limits.

(i) $f(x) = e^x$ with $S = e^1 - 1$:
One sees that the error rapidly decreases reaching the float precision limited region after five iterations in the Neville scheme. It follows the theoretical behavior which is of order $\mathcal{O}(h_i^{2i+2})$ to some extend as can be seen by comparison with the blue dashed-dotted curve. The deviation suggests that the error has other i-dependent contributions.

(ii) $f(x) = \sin^4(8x)$ with $S = \frac{3\pi}{4}$:
The error stays constant for a couple of iteration before decreasing with a similar rate compared to $f(x) = e^x$. Former behavior occurs because the number of samples does not suffice to resolve the oscillation period of the function which has an angular frequency of $\omega = 16$. As one can see, the error starts to decrease for $i > 5$ which corresponds to a sampling rate expressed in terms of angular frequency of

$$\omega_s(i) = \frac{2\pi}{h_i} = \frac{2\pi}{2\pi/2^i} = 2^i > 32 = 2^5 = 2\omega$$

This seems to correspond the Nyquist-Shanon sampling theorem.

(iii) $f(x) = \sqrt{x}$ with $S = \frac{2}{3}$:
Compared to the other functions, the error decreases noticeably slower for $f(x) = \sqrt{x}$. A possible explanation might be its diverging derivatives at $x = 0$, similar to the trapezoidal rule where the error depends on the first derivative at the integration boundaries. This argument is reaffirmed by the result after shifting the integration boundaries by $+1$ (dashed orange curve). Here, the error falls much more rapidly and dives into the unresolvable region at around $i = 7$.