Prof. Dr. Jens Honore Walther
Dr. Georgios Arampatzis
ETH Zentrum, CLT
CH-8092 Zürich

Solution Set 6

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Question 1: Simpson's rule from Newton–Cotes formulas

a) Setting $x_0 = a$, $x_1 = (a+b)/2$, $x_2 = b$, the Lagrange polynomials for $n = 2$ are given by

$$
\begin{aligned}
l_0^2 &= \frac{(x-(a+b)/2)(x-b)}{(a-(a+b)/2)(a-b)},\\
l_1^2 &= \frac{(x-a)(x-b)}{((a+b)/2-a)((a+b)/2-b)},\\
l_2^2 &= \frac{(x-(a+b)/2)(x-a)}{(b-(a+b)/2)(b-a)}.
\end{aligned} \tag{1}
$$

Using the Newton–Cotes formulas for $n = 2$,

$$
C_k^2 = \frac{1}{b-a}\int_a^b l_k^2(x)dx, \quad k = 0, 1, 2, \tag{2}
$$

the coefficient C_0^2 is computed by plugging in l_0^2 from (1) to (2):

$$
\begin{aligned}
C_0^2 &= \frac{1}{b-a}\int_a^b \frac{(x-(a+b)/2)(x-b)}{(a-(a+b)/2)(a-b)}\,dx\\
&= -\frac{1}{(b-a)^2}\frac{1}{a-(a+b)/2}\int_a^b (x-(a+b)/2)(x-b)\,dx\\
&= -\frac{1}{(b-a)^2}\frac{2}{a-b}\int_a^b x^2 - bx - \frac{1}{2}(a+b)x + \frac{1}{2}(a+b)b\,dx\\
&= \frac{1}{(b-a)^3}\int_a^b 2x^2 - ax - 3bx + ab + b^2\,dx\\
&= \frac{1}{(b-a)^3}\left(\frac{2}{3}x^3 - \frac{1}{2}ax^2 - \frac{3}{2}bx^2 + abx + b^2x\Big|_a^b\right)\\
&= \frac{1}{(b-a)^3}\left(\frac{2}{3}b^3 - \frac{1}{2}ab^2 - \frac{3}{2}b^3 + ab^2 + b^3 - \frac{2}{3}a^3 + \frac{1}{2}a^3 + \frac{3}{2}a^2b - a^2b - ab^2\right)\\
&= \frac{1}{(b-a)^3}\left(\frac{1}{6}(b^3-a^3) - \frac{1}{2}ab(b-a)\right)\\
&= \frac{1}{(b-a)^2}\left(\frac{1}{6}(b^2+ab+a^2) - \frac{1}{2}ab\right) = \frac{1}{(b-a)^2}\frac{1}{6}(b-a)^2 = \frac{1}{6}.
\end{aligned} \tag{3}
$$

Using property $C_k^n = C_{n-k}^n$ we obtain $C_2^2 = C_0^2 = 1/6$, and then using property

$$\sum_{k=0}^{n} C_k^n = 1, \tag{4}$$

we obtain

$$C_1^2 = 1 - C_0^2 - C_2^2 = 1 - \frac{1}{6} - \frac{1}{6} = \frac{2}{3}. \tag{5}$$

b) With the computed coefficients C_0^2, C_1^2 and C_2^2 from subquestion a, the resulting numerical integration rule using the Newton-Cotes formula is the Simpson's rule, which can be shown simply by :

$$I \approx (b-a) \sum_{k=0}^{2} C_k^2 f(x_k) = \frac{f(a) + 4f((a+b)/2) + f(b)}{6}(b-a). \tag{6}$$

Question 2: Trapezoidal and Simpson's rule

a) From the lecture notes we can use the equations 5.9 and 5.10 to simplify the calculation.

$$I \approx \frac{\Delta_x}{2} \left(f(x_0) + 2 \sum_{i=1}^{N-1} f(x_i) + f(x_N) \right) \tag{7}$$

$$I \approx \frac{\Delta_x}{3} \left(f(x_0) + 4 \sum_{\substack{i=1 \\ i=\text{odd}}}^{N-1} f(x_i) + 2 \sum_{\substack{i=2 \\ i=\text{odd}}}^{N-2} f(x_i) + f(x_N) \right) \tag{8}$$

By applying these formulas to the problem at hand, we get:

$$I \approx \frac{\pi}{12} \left(0 + 2 \left(\frac{1}{2} + \frac{\sqrt{3}}{2} + 1 + \frac{\sqrt{3}}{2} + \frac{1}{2} \right) + 0 \right) = \frac{\pi \left(2 + \sqrt{3}\right)}{6} \approx 1.9541 \tag{9}$$

for the trapezoidal rule and

$$I \approx \frac{\pi}{18} \left(0 + 4 \left(\frac{1}{2} + 1 + \frac{1}{2} \right) + 2 \left(\frac{\sqrt{3}}{2} + \frac{\sqrt{3}}{2} \right) + 0 \right) = \frac{\pi \left(8 + 2\sqrt{3}\right)}{18} \approx 2.000863 \tag{10}$$

for the Simpson's rule.

b) The exact value of the integral is obtained by performing the integration.

$$I = \int_0^{\pi} \sin(x) \, \mathrm{d}x = [-\cos(x)]_0^{\pi} = 2 \tag{11}$$

The absolute error of the trapezoidal rule is therefore $E_T = |2 - 1.9541| = 0.0459$ and the error of the Simpson's rule is $E_S = |2 - 2.000863| = 0.000863$. The Simpson's rule managed to get a more accurate result than the trapezoidal rule with the same amount of function evaluations. This is especially valuable when the cost to evaluate the function rises.

Question 3: Order of convergence

a) When considering $N-1$ intervals, where N is the number of data points, the error of the single intervals accumulate. If the applied integration rule has an error that scales as $\mathcal{O}(h^n)$, the accumulated error can be expressed as:

$$E = \sum_{i=1}^{N-1} c_i\, \mathcal{O}(h^n) \leq (N-1)\, \mathsf{max}(c_i)\, \mathcal{O}(h^n)\,, \tag{12}$$

where large sample sizes $N-1$ can be approximated with N and expressed as $N = \frac{b-a}{h}$. By applying this relation, the obtained order over a domain with multiple intervals is:

$$E \leq (b-a)\, \mathsf{max}(c_i)\, \mathcal{O}(h^{n-1}). \tag{13}$$

Therefore, the order of convergence is reduced by one order when considering multiple intervals. From the lecture notes we know that in a single interval, the rectangular rule converges with order 2, trapezoidal with order 3 and Simpson's rule with order 5 (see lecture notes, Eq.5.21, Eq.5.25 and Eq.5.27 respectively). Therefore, we are expecting the composite integration over a domain of multiple integrals to converge with order 1 for rectangular, order 2 for trapezoidal and order 4 for Simpson's rule with regards to the interval size.

b) By inspecting the graph, we observe that plot A decays with fourth order with respect to the interval size, plot B decays with second order and plot C with first order. We can conclude, keeping in mind the previous subquestion, that plot A corresponds to the Simpson's rule, plot B to the trapezoidal rule and plot C to the rectangular rule.

c) A higher order rule can perform worse than a lower order rule, if the constant factor (C_1) in the error of the higher order rule is greater than the factor (C_2) of the lower order rule. In that case it can be that $C_1 * h^n > C_2 * h^m$ for $m < n$ and $h << 1$. An example is given below in Fig. 1, where there is a point, where the Trapezoidal rule outperforms the Simpson's rule. (Also, if interested, have a look and "play" with the toy code we provided, in order to find other exemptions to the rule.

d) Through the previous question we know that the order of convergence over a whole domain with the Simpson's rule is fourth order accurate and second order for the trapezoidal rule. We can therefore express the errors in the following manner:

$$E_T = c_1\, \mathcal{O}(h^2) = c_1\, \mathcal{O}\left(\left(\frac{b-a}{N_1}\right)^2\right) \tag{14}$$

$$E_S = c_2\, \mathcal{O}(h^4) = c_2\, \mathcal{O}\left(\left(\frac{b-a}{N_2}\right)^4\right) \tag{15}$$

By inspection we can determine that to decrease the error by a factor of 1'000 we require $N_1^* = \sqrt{1'000}N_1 \approx 31.62N_1$ and $N_2^* = \sqrt[4]{1'000}N_2 \approx 5.62N_2$ more data points. We see that the Simpson's rule scales more efficiently than the trapezoidal rule.

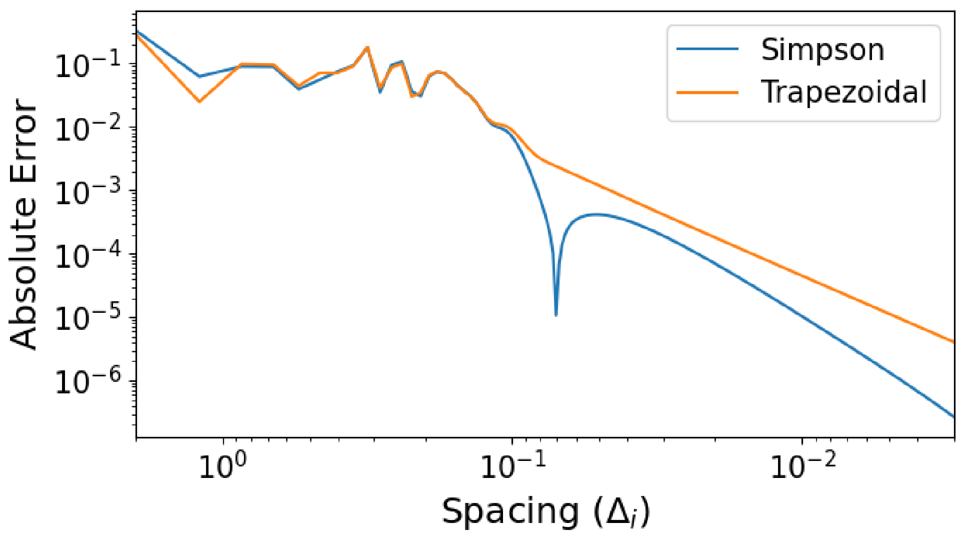

Figure 1: Error of Trapezoidal and Simpson's integration rule for numerical integration of the function $f(x) = \cos(\sin(\exp(x)))$ for varying interval sizes.