Numerical Methods 4H Assignment 1 - Adaptive Quadrature

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0.1 Question 1

Showing the error of the Simpson's rule is:

$$E(f;a,b) = -\frac{(b-a)^5}{2880} f^{iv}(c), for\ some\ c \in [a,b]$$

Consider the Taylor expansion about the mid point $c = (a+b)/2$. Let $h = b-a$, then $a = c{-}h/2$ and $b = c + h/2$.

$$\begin{aligned} f(a) &= f(c - \frac{h}{2}) \\ &= f(c) - \frac{h}{2}f'(c) + \frac{h^2}{8}f''(c) - \frac{h^3}{48}f'''(c) + \frac{h^4}{384}f^{(iv)}(c) + O(h^5) \end{aligned} \tag{1}$$

$$\begin{aligned} f(b) &= f(c + \frac{h}{2}) \\ &= f(c) + \frac{h}{2}f'(c) + \frac{h^2}{8}f''(c) + \frac{h^3}{48}f'''(c) + \frac{h^4}{384}f^{(iv)}(c) + O(h^5) \end{aligned} \tag{2}$$

$$\begin{aligned} f(x) &= f(c + (x-c)) \\ &= f(c) + (x-c)f'(c) + \frac{(x-c)^2}{2!}f''(c) + \frac{(x-c)^4}{4!}f^{(iv)}(c) + O(h^5) \end{aligned} \tag{3}$$

Substitute $x = c + uh/2$ into (3) and integrate (3) term by term, then

$$M(f) = \int_a^b f(x)\,\mathrm{d}x. = hf(c) + \frac{h^3}{24}f''(c) + \frac{h^5}{1920}f^{(iv)}(c) + O(h^7)$$

Let N(f,h) be the discretization method that approximates M(f). In this case it will be Simpson's rule:

$$N(f,h) = \frac{h}{6}(f(a) + 4f(c) + f(b))$$

Substitute (1) and (2) into N(f,h):

$$\begin{aligned} N(f,h) &= \frac{h}{6}[6f(c) + \frac{h^2}{4}f''(c) + \frac{h^4}{192}f^{(iv)}(c) + O(h^6)] \\ &= hf(c) + \frac{h^3}{24}f''(c) + \frac{h^5}{1152}f^{(iv)}(c) + O(h^7) \end{aligned}$$

We can now calculate the Error E(h):

$$
\begin{aligned}
E(h) &= M(f) - N(f,h) \\
&= \frac{h^5}{1920} f^{(iv)}(c) - \frac{h^5}{1152} f^{(iv)}(c) + O(h^7) \\
&= h^5 f^{(iv)}(c)(\frac{1}{1920} - \frac{1}{1152}) \\
&= \frac{-h^5 f^{(iv)}(c)}{2880} \\
&= \frac{-(b-a)^5 f^{(iv)}(c)}{2880}
\end{aligned}
$$

as required.

0.2 Question 2

Deriving Simpsons' Composite Rule

We'll generate N equal sub-intervals of [a,b], for some N $\in \mathbb{N}$
Label the sub-intervals as I_i with end-points $[x_{2i-2}, x_{2i}]$, for i = 1,...,N
The intervals are of equal length $x_{2i} - x_{2i-2} = 2h = \frac{(b-a)}{N}$
Where there are 2N + 1 quadrature points $x_i = a + ih$, i = 0,...,2N

Then the simpson rule on I_i is:

$$\begin{aligned}
\int_{I_i} f(x)\,\mathrm{d}x. &= \frac{2h}{6}(f(x_{2i-2}) + 4f(\frac{x_{2i-2} + x_{2i}}{2}) + f(x_{2i})) \\
&= \frac{h}{3}(f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i}))
\end{aligned}$$

and the sum of integrals over the sub-intervals is:

$$\begin{aligned}
\int_a^b f(x)\,\mathrm{d}x. &\approx \sum_{i=1}^{N} \int_{I_i} f(x) \\
&= \sum_{i=1}^{N} \frac{h}{3}(f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})) \\
&= \frac{h}{3} \sum_{i=1}^{N}(f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})) \\
&= \frac{h}{3}(f(x_0) + f(x_{2N}) + 2\sum_{i=1}^{N-1} f(x_{2i}) + 4\sum_{i=1}^{N} f(x_{2i-1}))
\end{aligned}$$

0.3 Question 3

Deriving the error in the Composite Simpson's rule $S_c(f; a, b, N)$

$$E_c(f; a, b, N) = -\frac{(b-a)^5}{2880N^4} f^{iv}(c), \ \ for\ some\ c \in [a, b]$$

It is not possible to derive the Composite Simpsons' error with only the information on the error for the normal Simpsons' rule. The Composite Simpson's rule performs the Simpson's rule on multiple sub-intervals meaning the error would be the sum of the errors of the ordinary Simpsons' rule on each sub-inverval. But since $f^{iv}(c)$ must be a different value of c for each interval; there is not enough information to combine these error intervals to derive the composite error.

For the jth node, $x_j = a + jh, \ j \in [0, 2N]$,
Expanding $f(x_j)$ using the Taylor Expansion gives the following:

$$f(x_j) = f(a+jh) = f(a)+jhf'(a)+\frac{(jh)^2}{2!}f''(a)+\frac{(jh)^3}{3!}f'''(a)+\frac{(jh)^4}{4!}f^{(iv)}(a)+O(h^5) \tag{4}$$

Let x = a + uh, then $f(x)$ gives the following Taylor Expansion:

$$f(x) = f(a+uh) = f(a)+uhf'(a)+\frac{(uh)^2}{2!}f''(a)+\frac{(uh)^3}{3!}f'''(a)+\frac{(uh)^4}{4!}f^{(iv)}(a)+O(h^5) \tag{5}$$

Since we have 2N + 1 points, $u \in [0, 2N]$ integrating $f(x)$ gives the following:

$$\begin{aligned} M(f) &= \int_0^{2N} hf(a+uh)\,\mathrm{d}u. \\ &= h[uf(a) + \frac{u^2h}{2}f'(a) + \frac{u^3h^2}{6}f''(a) + \frac{u^4h^3}{24}f'''(a) + \frac{u^5h^4}{120}f^{(iv)}(a) + O(h^5)]_0^{2N} \\ &= 2Nhf(a) + 2(Nh)^2f'(a) + \frac{4(Nh)^3}{3}f''(a) + \frac{2(Nh)^4}{3}f'''(a) + \frac{4(Nh)^5}{15}f^{iv} + O(h^6) \end{aligned} \tag{6}$$

To solve for $E_c(f; a, b, N)$ we note that

$$S_c(f; a, b, N) = \frac{h}{3}(f(x_0) + f(x_{2N}) + 2\sum_{i=1}^{N-1} f(x_{2i}) + 4\sum_{i=1}^{N} f(x_{2i-1}))$$

substitute each term into the $f(xj)$ expansion (4), and then subtract the whole sum from M(f). This should result in the error value.

0.4 Question 4

Implementation of Composite Simpsons' rule in Matlab.

See file Sc.m for the same code as below.

```
function out = Sc(f, a, b, N)
% Sc(f, a, b, N)
% This function calculates the integral of f on the interval [a,b]
% using the Composite Simpson rule with N subintervals, the supplied N
% value should be even

    % Shorthand for double the ino of subintervals
    N2 = 2 * N;
    % Generate 2N + 1 equally spaced nodes
    points = linspace(a, b,  N2 + 1) ;

    % Evalulate f at each node
    fx = f(points);

    % Define the distance between each node
    h = ((b - a) / N2);

    % Apply the composite simpson rule
    odd_terms  =  sum(fx(2:2:N2));
    even_terms =  sum(fx(3:2:N2));
    out = (h/3.0) * (fx(1) + (2 * even_terms) + (4 * odd_terms) + fx(N2+1));

end
```

0.5 Question 5

Considering an interval [a,b] small enough to justify $f^{iv}(x) = const$ on [a,b]
Prove:

$$E(f;a,b,2) = \frac{1}{15}(S_c(f;a,b,2) - S_c(f;a,b,1)) \; and \; then \; \int_a^b f(x)\,\mathrm{d}x = S_c(f;a,b,2) + E(f;a,b,2)$$

Solution:

Note that:

$$\begin{aligned}
Sc(f;a,b,1) &= \frac{h}{3}(f(x_0) + f(x_2) + 2\sum_{i=1}^{0} f(x_{2i}) + 4\sum_{i=1}^{1} f(x_{2i-1})) \\
&= \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) \\
&= \frac{h}{3}(f(a) + 4f(\frac{a+b}{2}) + f(b)) \\
&= S(f;a,b)
\end{aligned}$$

$$\implies Ec(f;a,b,1) = E(f;a,b)$$

As f^{iv} is constant: $f^{(iv)}(c) = \alpha$ for $\forall c \in [a,b]$ where α is a constant
Then:

$$E(f;a,b) = -\frac{(b-a)^5}{2880}\alpha$$

$$E_c(f;a,b,2) = -\frac{(b-a)^5}{2880 * 2^4}\alpha$$

$$\implies E(f;a,b) = 16E_c(f;a,b,2)$$

Let $M(f) = \int_a^b f(x)\,\mathrm{d}x$

From definition of Numerical Schemes

$$\begin{aligned}
M(f) &= S_c(f;a,b,2) + E_c(f;a,b,2) \\
M(f) &= S_c(f;a,b,1) + E_c(f;a,b,1)
\end{aligned}$$

Then:

$$
\begin{aligned}
S_c(f;a,b,2) - S_c(f;a,b,1) &= M(f) - E_c(f;a,b,2) - M(f) + E_c(f;a,b,1) \\
&= E_c(f;a,b,1) - E_c(f;a,b,2) \\
&= E(f;a,b) - E_c(f;a,b,2) \\
&= 16E_c(f;a,b,2) - E_c(f;a,b,2) \\
&= 15E_c(f;a,b,2)
\end{aligned}
$$

$$
\iff \frac{1}{15}(S_c(f;a,b,2) - S_c(f;a,b,1)) = E_c(f;a,b,2)
$$

as required.

Let $E(f;a,b,2) = E_c(f;a,b,2)$ and by $M(f) = S_c(f;a,b,2) + E_c(f;a,b,2)$ it follows that:

$$
\int_a^b f(x)\,\mathrm{d}x = S_c(f;a,b,2) + E(f;a,b,2)
$$

0.6 Question 6

Implementation of Adaptive Simpsons' rule in Matlab.

See file Sa.m for the same code as below.

```
function out = Sa(f, a, b, eps)
% Sa(f, a, b, eps)
% This function calculates the integral of f on the interval [a,b]
% using the Adaptive Simpson rule with a given error (epsilon) value

    % Calculate mid-point c
    c = (a + b)/2;

    % Obtain first integral approximation using 3 nodes
    Q1  = Sc(f, a, b, 1);

    % Obtain second integral approximation using 5 nodes
    Q2 =  Sc(f, a, b, 2);

    % Estimate the error
    err = (Q2 - Q1) / 15.0;

    % Check if error estimate is less than the tolerance eps.
    % if it is, then Q2 is an appropriate estimate, and is returned.
    % Otherwise we split [a,b] into two equal subintervals and repeat
    % this process over each subinterval with tolerances adjusted to eps/2
    if abs(err) < eps
        out =  Q2;
    else
        out = Sa(f, a , c, eps/2.0) + Sa(f, c, b, eps/2.0);
    end
end
```

0.7 Question 7

Plotting $\int_0^2 sin(1 - 25erf(\frac{x-1}{0.2\sqrt{2}})\,\mathrm{d}x.$ at first with the adaptive simpsons rule with an error of 10^{-3} is evaluated at 133 unique points. Then plotting the same amount of points with 66 intervals of composite simpson's rule gives the following graphs for each. The '+' marks the points at which the function is evaluated at.

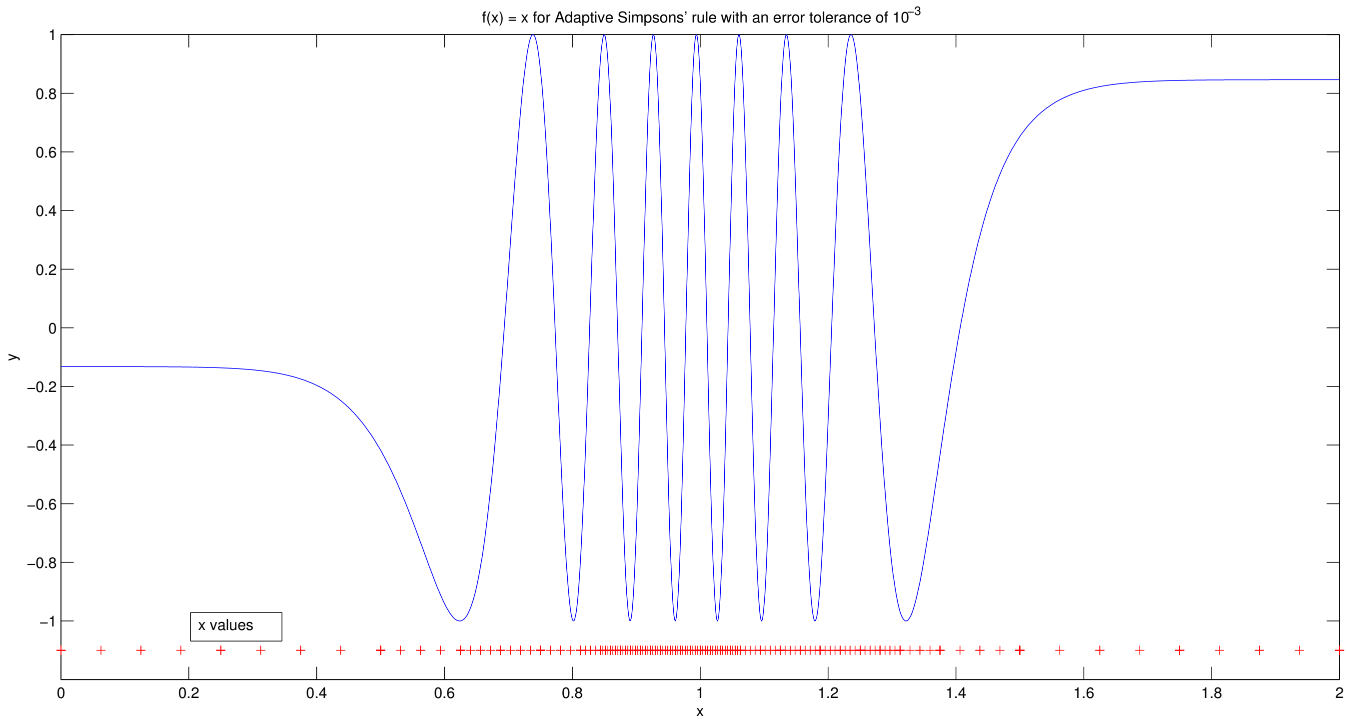

Figure 1: Adaptive Simpsons'

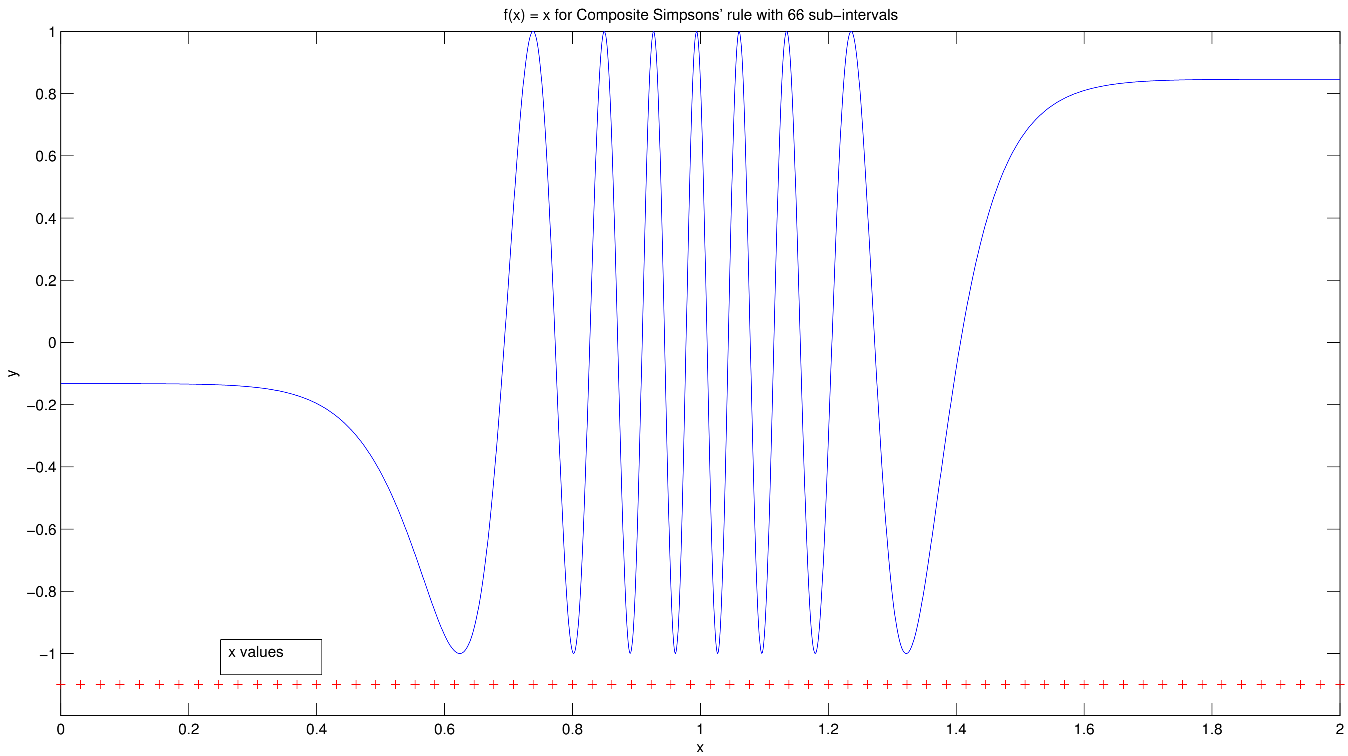

Figure 2: Composite Simpson'

As you can see for the Composite Simpsons' rule, the quadrature points are uniform. Whereas for the Adaptive Simpsons' rule the quadrature points are more around the centre. This makes sense as the error is likely to be larger where the graph isn't as 'regular', so the adaptive procedure tends towards those intervals.

0.8 Question 8

Plotting $\int_0^2 sin(1 - 25erf(\frac{x-1}{0.2\sqrt{2}}) \, \mathrm{d}x$. For the integral

$$I = \int_{-3}^{5} exp(-50(x-1)^2) \, \mathrm{d}x.$$

Taking 10 equally spaced error tolerance values ranging from 10^-6 to 10^-12 and applying them to the Adaptive Simpsons' function then working out absolute value of the difference between the results and the actual values; and applying this against the error tolerance values supplied gives the following graph:

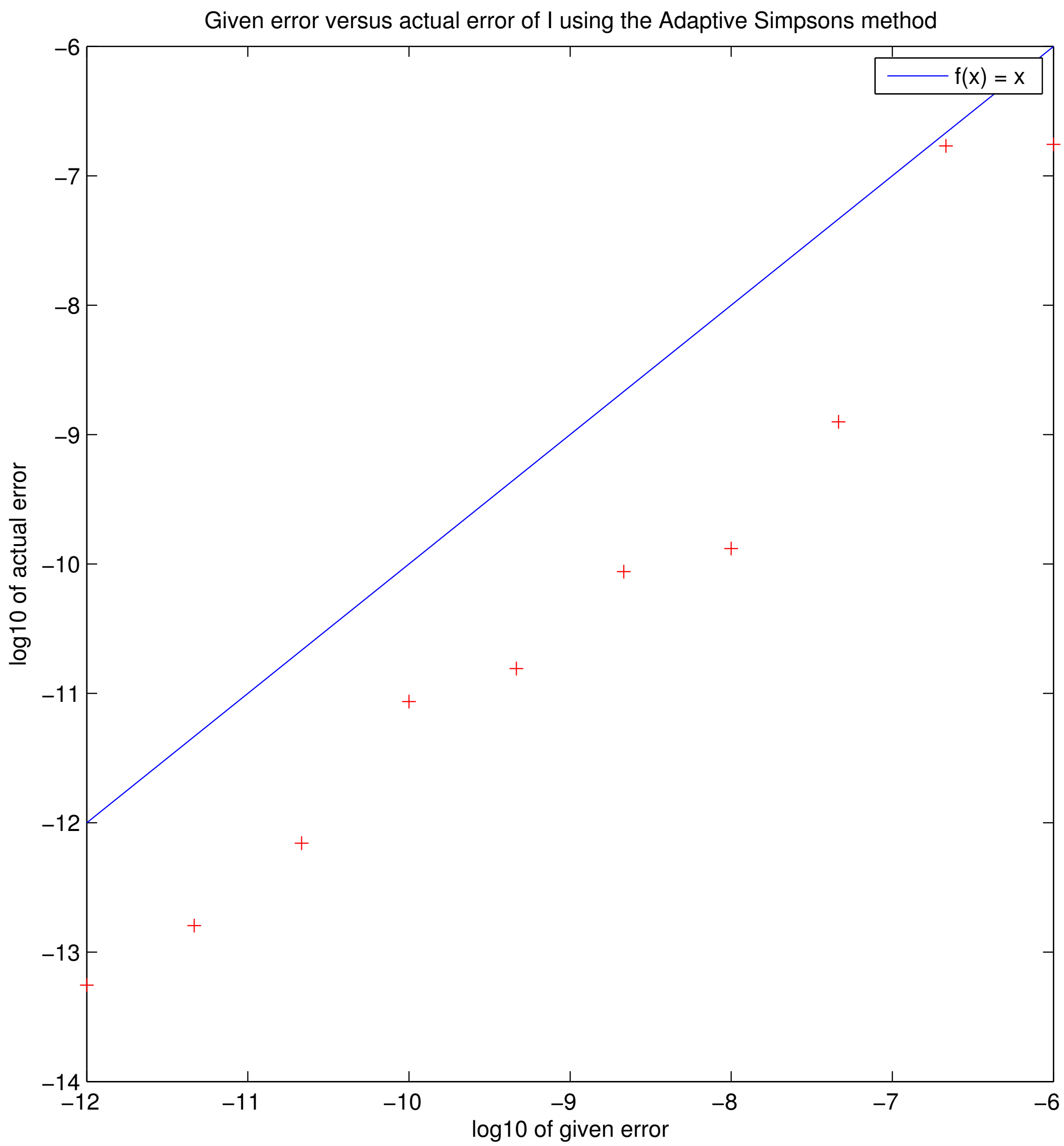

Figure 3: Adaptive Error'

The graph shows as expected as the Adaptive Simpsons' formula should give an error of equal to or less than that given to it. Which can be seen for all 10 points on the graph.