Question 1.b

Error is defined as $\Delta = I_e - I_r$, where e and r stands for estimated value and real value respectively. Here we have I_e = the integration that we have found by Simpson's method, I_r is the real integration.

For Simpson's method we take the integral,

$$I = \frac{h}{3}\left[f(a) + 4f(m) + f(b)\right]$$

Where a, b are endpoints, m is mid point

$m = \frac{a+b}{2}$, $h = \frac{b-a}{2}$

$$\Rightarrow I = \frac{h}{3}\left[f(a) + 4f(a+h) + f(b)\right]$$

Say, the real integration of a function $f(x)$ from 0 to x be $I_0(x) = \int_0^x f(x)dx$ [assume $f(0)=0$]

Then, the integration we intend to find is $\int_a^b f(x)\,dx = I_0(b) - I_0(a)$

$$\text{or, } I_0(b) - I_0(a) = \int_a^b f(x)\,dx$$

Now, we can write it by Taylor expansion around the point $x=a$ like this

$$I_0(b) - I_0(a) = I_0'(a)(b-a) + I_0''(a)\frac{(b-a)^2}{2!} + I_0'''(a)\frac{(b-a)^3}{3!} + \cdots$$

or, $$I_0(b) - I_0(a) = f(a)(2h) + f_0'(a)\frac{(2h)^2}{2!} + \cdots + f^{(n-1)}\frac{(2h)^n}{n!} + \cdots$$

Because, $I'(a) = f(a)$, $I''(a) = f'(a)$ and $I^{(n)}(a) = f^{(n-1)}(a)$ in general. (Here, $b-a = 2h$)

However, the approximated integral in Simpson's method is

$$I = \frac{h}{3}\left(f(a) + 4f(m) + f(b)\right)$$

or, $$I = \frac{h}{3}\left(f(a) + 4f(a+h) + f(a+2h)\right)$$

$$= \frac{h}{3}\left(f(a) + 4\left(f(a) + hf'(a) + \frac{h^2}{2!}f''(a) + \cdots\right) + \left(f(a) + (2h)f'(a) + f''(a)\frac{(2h)^2}{2!} + \cdots\right)\right)$$

or, $I = \frac{h}{3}\left[6f(a) + \sum_{n\geq 1} \frac{(4+2^n)h^n f^{(n)}(a)}{n!}\right]$

$$= (2h)f(a) + \frac{(2h)^2}{2!} f^{(1)}(a) + \frac{(2h)^3}{3!} f^{(2)}(a)$$
$$+ \frac{(2h)^4}{4!} f^{(3)}(a) + \frac{5}{18} h^5 f^{(4)}(a) + \cdots\cdots$$

So, the error is $\Delta = I - I_0$

or, $\Delta = \left[\frac{5}{18} h^5 - \frac{(2h)^5}{5!}\right] f^{(4)}(a) + O(h^6)$

$\frac{32}{120} = \frac{4}{15}$

$$= \left[\frac{5}{18} - \frac{4}{15}\right] h^5 f^{(4)}(a) + O(h^6)$$

$$= \frac{3}{270} h^5 f^{(4)}(a) + O(h^6)$$

$$= \frac{h^5}{90} f^{(4)}(a) + O(h^6)$$

Now, for n bins we have the error estimation as

$$\Delta_0 = n\Delta = \frac{(nh)\, h^4 f^{(4)}(a)}{90} + O(h^6)$$

Now, $nh = \frac{b-a}{2}$ e.g for $n=1$ we had $h = \frac{b-a}{2}$.

So, $\Delta_0 = \frac{(b-a)}{180} h^4 f^{(4)}(a)$

$$= \frac{(b-a)}{180}\left(\frac{b-a}{2n}\right)^4 f^{(4)}(a) \qquad \left[\text{as } h = \frac{b-a}{2n}\right]$$

$$= \frac{(b-a)^5 f^{(4)}(a)}{2880\, n^4}$$

neglecting higher order terms.

Now, this integration in the question has limits $a = 1$ and $b = 3$.

And, $f(x) = x(\ln(x) - 1)$

$\rightarrow f^{(1)}(x) = \ln(x)$, $f^{(2)}(x) = \frac{1}{x}$, $f^{(3)}(x) = -\frac{1}{x^2}$

and $f^{(4)}(x) = \frac{2}{x^3} \Rightarrow f^{(4)}(1) = 2$

$$\Rightarrow \Delta_0 = \frac{(b-a)^5}{1440 n^4}$$

The value we obtained by calculating the integral

was $I = -1.05624470020364$.

The exact integral we should get is

$$I_0 = \int_1^3 (x \ln x - x)\,dx = \frac{9 \log(9)}{4} - 6$$

$$\approx -1.05624470099351$$

$\Delta = I - I_0 \rightarrow |\Delta| \approx 7.898\ 7616 \times 10^{-10}$

Now, $b - a = 3 - 1 = 2$ while number of bins we have used is 100.

$$\Rightarrow \Delta = \frac{(b-a)^5}{1440 \times (100)^2} = 2.22 \times 10^{-10}$$

Hence, we can see that the order is same as found from the numerical calculation.