Simpson Rule - Solutions

1. We must evaluate
$$\int_0^{\pi/2} e^{\sin x} dx$$
to an accuracy of $\varepsilon = 10^{-5}$ using the Composite Simpson's Rule. The error term for the Composite Simpson's Rule gives
$$|\Delta| = \frac{h^4}{180}\left(\frac{\pi}{2} - 0\right) K \leqslant \varepsilon = 10^{-5}$$
where
$$K = \max_{0 \leqslant x \leqslant \pi/2} \left|f^{(4)}(x)\right|.$$
Here, $f(x) \equiv e^{\sin x}$. We find
$$f^{(4)}(x) = e^{\sin x}\left(\cos^4 x - 4\cos^2 x - 6\cos^2 x \sin x + 3\sin^2 x + \sin x\right).$$
This gives $\left|f^{(4)}(0)\right| = 3$ and $\left|f^{(4)}\left(\frac{\pi}{2}\right)\right| = 4e$. Using Newton's Method we also find that $\left|f^{(4)}(x)\right|$ has a maximum at $x = 0.4716$. However, $\left|f^{(4)}(0.4716)\right| = 5.7244$. Hence,
$$K = \left|f^{(4)}\left(\frac{\pi}{2}\right)\right| = 4e = 10.873127$$
From the error expression we then obtain
$$h^4 \leqslant 0.00010539 \Rightarrow h \leqslant 0.10132102.$$
Since $h = \frac{b-a}{2N}$ for the Composite Simpson's Rule (in this example, $a = 0$ and $b = \frac{\pi}{2}$), we have
$$\begin{aligned} \frac{\frac{\pi}{2} - 0}{2N} &\leqslant 0.10132102 \\ &\Rightarrow N \geqslant 7.75 \\ &\Rightarrow N = 8 \\ &\Rightarrow h = \frac{\frac{\pi}{2} - 0}{16} = 0.098175 \end{aligned}$$

This generates the discrete data

i	0	1	2	3	4	5	6	7	8
x_i	0	0.0982	0.1963	0.2945	0.3927	0.4909	0.5890	0.6872	0.7854
$f(x_i)$	1	1.1030	1.2154	1.3368	1.4662	1.6022	1.7429	1.8859	2.0281

i	9	10	11	12	13	14	15	$16 = 2N$
x_i	0.8836	0.9817	1.0799	1.1781	1.2763	1.3744	1.4726	$1.5708 = \frac{\pi}{2}$
$f(x_i)$	2.1663	2.2967	2.4155	2.5190	2.6037	2.6665	2.7052	2.7183

The Composite Simpson's Rule gives

$$\begin{aligned}
\int_0^{\pi/2} e^{\sin x} dx &\simeq \frac{h}{3}\left[f(x_0) + f(x_{2N}) + 4\sum_{i=0}^{N-1} f(x_{2i+1}) + 2\sum_{i=1}^{N-1} f(x_{2i})\right] \\
&= \frac{0.098175}{3}[1 + 2.7183 \\
&\quad +4\,(1.1030 + 1.3368 + 1.6022 + 1.8859 + 2.1663 + 2.4155 + 2.6037 + 2.7052) \\
&\quad +2\,(1.2154 + 1.4662 + 1.7429 + 2.0281 + 2.2967 + 2.5190 + 2.6665)] \\
&= 3.10437901
\end{aligned}$$

The result obtained with $N = 500000$ (representing an accuracy of about 10^{-24}) is 3.10437902. We will regard this value as the true value due to the very high degree of accuracy. Thus,

$$|3.10437902 - 3.10437901| = 2 \times 10^{-8}$$

which is definitely less than the required accuracy of 10^{-5}, indicating that the integral has been successfully evaluated to within the specified accuracy. Note that we have worked to a precision of 15 decimal places in this problem, even though we have presented the values to a lesser precision (we present them to a lesser precision to avoid having the whole page covered with numbers).

2. Here, we evaluate

$$\int_0^1 e^{-e^{-x}} dx$$

using the Composite Simpson's Rule with $N = 5$.

For h we have

$$h = \frac{1-0}{2N} = \frac{1}{10} = 0.1$$

which results in the discrete data $\left(f(x_i) \equiv e^{-e^{-x_i}}\right)$

i	0	1	2	3	4	5
x_i	0	0.1	0.2	0.3	0.4	0.5
$f(x_i)$	0.3679	0.4046	0.4410	0.4767	0.5115	0.5452

i	6	7	8	9	10
x_i	0.6	0.7	0.8	0.9	1.0
$f(x_i)$	0.5776	0.6086	0.6381	0.6659	0.6922

.

Applying the Composite Simpson's Rule gives

$$\begin{aligned}\int_0^{\pi/2} e^{-e^{-x}} dx &\simeq \frac{h}{3}\left[f(x_0) + f(x_{10}) + 4\sum_{i=0}^{4} f(x_{2i+1}) + 2\sum_{i=1}^{4} f(x_{2i})\right] \\ &= 0.5400320\end{aligned}$$

The result obtained using $N = 500000$ is 0.5400319, suggesting that the above value is accurate to 6 decimal places.

3. Here, we evaluate

$$\int_0^1 \frac{\sin x}{x} dx$$

using the Composite Simpson's Rule with $N = 5$.

For h we have

$$h = \frac{1-0}{2N} = \frac{1}{10} = 0.1$$

which results in the discrete data $\left(f(x_i) \equiv \frac{\sin x}{x}\right)$

i	0	1	2	3	4	5
x_i	0	0.1	0.2	0.3	0.4	0.5
$f(x_i)$	1	0.9983	0.9933	0.9850	0.9735	0.9588

i	6	7	8	9	10
x_i	0.6	0.7	0.8	0.9	1.0
$f(x_i)$	0.9410	0.9203	0.8966	0.8703	0.8414

.

Note the application of L'Hôpital's rule at x_0 $\left(\lim\limits_{x\to 0} \frac{\sin x}{x} = 1\right)$.

Applying the Composite Simpson's Rule gives

$$\begin{aligned}\int_0^{\pi/2} \frac{\sin x}{x} dx &\simeq \frac{h}{3}\left[f(x_0) + f(x_{10}) + 4\sum_{i=0}^{4} f(x_{2i+1}) + 2\sum_{i=1}^{4} f(x_{2i})\right] \\ &= 0.9460832\end{aligned}$$

The result obtained using $N = 500000$ is 0.9460831, suggesting that the above value is accurate to 6 decimal places.

4.

$$\begin{aligned} f(x) &\equiv xe^x \\ f'(x) &= xe^x + e^x \\ f''(x) &= xe^x + 2e^x \\ f'''(x) &= xe^x + 3e^x \\ f^{(4)}(x) &= xe^x + 4e^x \\ f^{(5)}(x) &= xe^x + 5e^x = (x+5)e^x \end{aligned}$$

(a) Firstly, we determine the necessary stepsize h. To evaluate $\max|f^{(4)}(x)|$ we solve $f^{(5)}(x) = 0$ which yields $x = 5 \notin [-1, 1]$. At the boundaries we have

$$|f^{(4)}(x = -1)| = 3e^{-1} \approx 1.103638$$

and

$$|f^{(4)}(x = 1)| = 5e \approx 13.591409.$$

So the maximum K is $5e$.

1. Thus, we must satisfy

$$\frac{h^4}{180}(b-a)\cdot K = \frac{h^4}{180}(1-(-1))\cdot 5e < 0.001$$

with

$$h < \sqrt{\sqrt{\frac{0.036}{e}}} = 0.3392361, \qquad n = \frac{b-a}{2h} > \frac{b-a}{2\times 0.3392361}.$$

Consequently

$$n = \left\lceil \frac{1-(-1)}{2 \times 0.3392361} \right\rceil = 3.$$

and

$$h = \frac{b-a}{2n} = \frac{1}{3}.$$

(b)

1.

j	x_j	$factor$	$factor \times f(x_j)$
0	-1	1	-0.367879441
1	$-\frac{2}{3}$	4	-1.369112317
2	$-\frac{1}{3}$	2	-0.477687540
3	0	4	0
4	$\frac{1}{3}$	2	0.930408283
5	$\frac{2}{3}$	4	5.193957443
6	1	1	2.718281828
			sum = 6.6279682560

In this table, $factor$ refers to the coefficients in the Composite Simpson's Rule

$$\int_{-1}^{1} xe^x dx \approx \frac{h}{3}\left[f(x_0) + f(x_6) + 4\sum_{i=0}^{2} f(x_{2i+1}) + 2\sum_{i=1}^{2} f(x_{2i})\right].$$

Hence,

$$\int_{-1}^{1} xe^x dx \approx \left(\frac{1}{9}\right) 6.627968256 = 0.736440917.$$

Comparing to the analytical result

$$\int_{-1}^{1} xe^x = \frac{2}{e}$$

we find

$$\left|\frac{2}{e} - 0.736440917\right| \approx 0.000682$$

which is more than the accuracy we required.

5. The error in Simpson's Rule on the interval I satisfies

$$\Delta \leqslant \frac{h^5}{90} \max_I \left| f^{(4)}(x) \right| .$$

If $f(x) = ax^3 + bx^2 + cx + d$, then

$$f^{(4)}(x) = 0$$

and so

$$\Delta = 0$$

which means that Simpson's Rule is exact when $f(x) = ax^3 + bx^2 + cx + d$.

6. Firstly we note that the expression for the maximum error in the Composite Simpson's Rule

$$|\Delta| = \frac{h^4}{180}(1 - (-1)) M$$

contains the term

$$M = \max_{[-1,1]} \left| \frac{d^4}{dx^4} \left(e^{-x^2} - \frac{1}{e} \right) \right| .$$

We have

$$\begin{aligned} y^{(5)} &= \frac{dy^{(4)}}{dx} = \frac{d}{dx}\left(e^{-x^2}\left(12 - 48x^2 + 16x^4\right)\right) \\ &= e^{-x^2}\left(-120x + 160x^3 - 32x^5\right) \end{aligned}$$

and, to find the stationary points of $y^{(4)}$,

$$\begin{aligned} y^{(5)} = 0 \;\; &\Rightarrow \;\; e^{-x^2}\left(-120x + 160x^3 - 32x^5\right) = 0 \\ &\Rightarrow \;\; -120x + 160x^3 - 32x^5 = 0 \\ &\Rightarrow \;\; 120x - 160x^3 + 32x^5 = 0 \\ &\Rightarrow \;\; x = \pm 0.9586 \text{ and } 0. \end{aligned}$$

So we have

$$\begin{aligned} \left| y^{(4)}(-1) \right| &= 7.3576 \\ \left| y^{(4)}(-0.9586) \right| &= 7.4195 \\ \left| y^{(4)}(0) \right| &= 12 \\ \left| y^{(4)}(0.9586) \right| &= 7.4195 \\ \left| y^{(4)}(1) \right| &= 7.3576 \end{aligned}$$

The first and last of these are $\left|y^{(4)}\right|$ at the endpoints of the interval. Clearly, the maximum of $\left|y^{(4)}\right|$ is 12

We now find an upper bound for h

$$\begin{aligned} |\Delta| &= \frac{h^4}{180}(1-(-1))\,12 \leqslant \varepsilon = 10^{-3} \\ &\Rightarrow h \leqslant 0.294287 \end{aligned}$$

This gives

$$\begin{aligned} h &= \frac{1-(-1)}{2N} \leqslant 0.294287 \\ &\Rightarrow N \geqslant 3.398 \Rightarrow N = 4 \end{aligned}$$

and this gives the actual value of h that must be used

$$h = \frac{1-(-1)}{2N} = 0.25$$

We thus have the discrete data

i	0	1	2	3	4	5	6	7	8
x_i	-1	-0.75	-0.5	-0.25	0	0.25	0.5	0.75	1
$f(x_i)$	0	0.2019	0.4109	0.5715	0.6321	0.5715	0.4109	0.2019	0

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The Composite Simpson's Rule gives

$$\begin{aligned} \int_{-1}^{1}\left(e^{-x^2}-\frac{1}{e}\right)dx &\approx \frac{h}{3}\left[f(x_0)+f(x_8)+4f(x_1)+\sum_{k=1}^{3}2f(x_{2k})+4f(x_{2k+1})\right] \\ &= 0.75795. \end{aligned}$$

The exact value is

$$\int_{-1}^{1}\left(e^{-x^2}-\frac{1}{e}\right)dx = \left[\frac{\sqrt{\pi}}{2}\operatorname{erf}(x)-\frac{x}{e}\right]_{-1}^{1} = 0.75788938..$$

so that

$$|0.75788938.. - 0.75795| = 6\times 10^{-5} < \varepsilon$$

and the integral has been evaluated to the required degree of accuracy.

7.