

problem	exact	Trapezoidal	Simpson
(a)	0.386294...	0.346573...	0.385834...
(b)	0.0348119...	0.0232079...	0.0322961...
(c)	0.307092...	0.392699...	0.305432...

Single interval Trapezoidal rule and error term is

$$\int_a^b f(x) = \frac{h}{2}(f(a) + f(b)) - \frac{h^3}{12}f''(\zeta), \quad h = b - a,$$

for some ζ between a and b . The error satisfies

$$|\text{error}| \leq \frac{h^3}{12} \max_{a \leq \zeta \leq b} |f''(\zeta)|$$

The actual error (exact - approximate solution) must be less than or equal to this upper bound.

Upper bound for the trapezoidal Rule error in the three cases is:

$$(a) |\text{error}| \leq \frac{h^3}{12} \max_{1 \leq \zeta \leq 2} |-\zeta^{-2}| = \frac{1}{12},$$

$$(b) |\text{error}| \leq \frac{0.1^3}{12} \max_{0 \leq \zeta \leq 0.1} |2/9\zeta^{-5/3}| = \infty \text{ unbounded}$$

$$(c) |\text{error}| \leq \frac{\pi^3}{27 \times 12} \max_{0 \leq \zeta \leq \pi/3} |4 \cos^2(\zeta) - 2| = \frac{\pi^3 \times 2}{27 \times 12}.$$

The Simpson Rule results are similar, but use the 4th derivative.

Question 2

problem	exact	Trapezoidal	Simpson	Midpoint	Open NC 2f's
(a)	0.102459...	0.102440...	0.102459...	0.102469...	0.102466...
(b)	0.785398...	0.785398...	0.785398...	0.785398...	0.785398...
(c)	0.75	0.5	0.695800...	0.793700...	0.783470...

The second and fourth derivatives are used in the various error estimates. The idea is to work them out and find their maximum value over the range of integration.

$$(a) \quad f(x) = \sqrt{1+x}, \quad |f''(x)| = \left| \frac{-1}{4(1+x)^{3/2}} \right| \leq \frac{1}{4}, \quad |f^{(4)}(x)| = \left| \frac{-15}{16(1+x)^{7/2}} \right| \leq \frac{15}{16}.$$

$$(b) \quad f(x) = \sin^2(x), \quad |f''(x)| = |4 \cos^2(x) - 2| \leq 2, \quad |f^{(4)}(x)| = |-16 \cos^2(x) + 8| \leq 8.$$

$$(c) \quad f(x) = x^{1/3}, \quad |f''(x)| = \left| \frac{-2}{9x^{5/3}} \right| \leq \infty, \quad |f^{(4)}(x)| = \left| \frac{-80}{81x^{11/3}} \right| \leq \infty.$$

The maximum errors in the schemes are given below. The actual errors are all smaller than these values and hence are consistent with them.

problem	Trapezoidal	Simpson	Midpoint	Open NC 2f's
(a)	2×10^{-5}	3×10^{-9}	1×10^{-5}	7×10^{-6}
(b)	0.645...	0.0265...	0.322...	0.215...
(c)	∞	∞	∞	∞

Question 3

Following the notes and the Simpson Rule handout we find that

$$\int_a^b f(x)dx = 3hf(c) + \frac{9h^3}{8}f''(c) + O(h^5)$$

where $c = (a+b)/2$ is the midpoint and $h = b-a$. The next stage is to rewrite the approximation in terms of c and h :

$$\text{approx} = \frac{3h}{2}(f(a+h) + f(a+2h)) = \frac{3h}{2}(f(c-h/2) + f(c+h/2)) .$$

Next Taylor expand about $h = 0$ to get

$$\frac{3h}{2}(f(c-h/2) + f(c+h/2)) = 3hf(c) + \frac{3h^3}{8}f''(c) + O(h^5).$$

Finally, subtract the two Taylor expansions at the same place to get

$$\text{exact} - \text{approximate} = \frac{3h^3}{4}f''(c) + O(h^5)$$

The other scheme can be rewritten in terms of c and h as:

$$\text{approx} = \frac{3h}{8}(f(c-3h/2) + f(c+3h/2)) + \frac{9h}{8}(f(c-h/2) + f(c+h/2)) .$$

Taylor expand about $h = 0$ to get eventually

$$3hf(c) + \frac{9h^2}{8}f''(c) + \frac{21h^5}{128}f^{(iv)}(c) + O(h^7)$$

Exact is obtained as for first part, but we need the next nonzero term in the series also

$$\int_a^b f(x)dx = 3hf(c) + \frac{9h^3}{8}f''(c) + \frac{81h^5}{640}f^{(iv)}(c) + O(h^7)$$

Finally, subtracting the two Taylor expansions at the same place to get

$$\text{exact} - \text{approximate} = \frac{-3h^5}{80}f^{(iv)}(c) + O(h^7)$$

Question 4

with $b = a + 3h$, $h = (b-a)/3$, we have

$f(x)$	$\int_a^b f(x)dx$	Approximation	Match
1	$b-a$	$b-a$	yes
x	$b^2/2 - a^2/2$	$\frac{3h}{8}(8a+12h)$	yes
x^2	$b^3/3 - a^3/3$	$\frac{3h}{8}(a^2 + 3(a+h)^2 + 3(a+2h)^2 + (a+3h)^2)$	yes
x^3	$b^4/4 - a^4/4$	$\frac{3h}{8}(a^3 + 3(a+h)^3 + 3(a+2h)^3 + (a+3h)^3)$	yes
x^4	$b^5/5 - a^5/5$	$\frac{3h}{8}(a^4 + 3(a+h)^4 + 3(a+2h)^4 + (a+3h)^4)$	no

The degree of precision is 3. Check for yourselves that the two columns are the same up to the x^3 terms.

The mismatch in the last case is $-9h^5/10$. This can be verified in the special case $a = 0, b = 1$ giving exact = $1/5$ approximate = $11/54$, error = $-1/270$. It doesn't match for this particular choice of a, b and so doesn't match in general. Maple is good at doing the algebra required for the other parts. It can also help to write $a = c - 3h/2$ and $b = c + 3h/2$ where $c = (a + b)/2$ and $h = (b - a)/3$ and do the whole thing in terms of c, h instead of a, b .

Substitute $f(x) = 1, x, x^2$ etc. in turn into the error term. The result is zero until a high enough power is substituted. In this case all results are zero until $f(x) = x^4$ which gives error = $-9h^5/10 = 4!\delta$, so $\delta = -3h^5/80$.

Question 5

Similar to the last one. Solve simultaneous equations for α, β, γ . (It will help to write $a = c - h$ and $b = c + h$ where $c = (a + b)/2$ and $h = (b - a)/2$ and do the whole thing in terms of c, h instead of a, b .)

$$\begin{aligned}\alpha + \beta + \gamma &= 2h \\ a\alpha + (a + h)\beta + (a + 2h)\gamma &= 2ah + 2h^2 \\ a^2\alpha + (a + h)^2\beta + (a + 2h)^2\gamma &= 2a^2h + 4ah^2 + 8/3h^3 \\ a^3\alpha + (a + h)^3\beta + (a + 2h)^3\gamma &= 2a^3h + 6a^2h^2 + 8ah^3 + 4h^4\end{aligned}$$

solving (quicker using Maple, or transforming to a variable where $a = 0$) gives

$$\alpha = \frac{h}{3}, \quad \beta = \frac{4h}{3}, \quad \gamma = \frac{h}{3},$$

and the final substitution $f(x) = x^4$ gives $\delta = -h^5/90$. This is Simpson's Rule (see handout).

Question 6

problem	exact	Trapezoidal	Simpson	Midpoint
(a)	1.098612...	1.116666...	1.098725...	1.089754...
(b)	4	4.25	4	3.875
(c)	0.636619...	0.622008...	0.636636...	0.643950...

Question 7

The Composite Midpoint Rule on $2n$ subintervals is

$$\text{approximate integral} = h \sum_{j=0}^{n-1} f(a + (2j + 1)h), \quad h = (b - a)/2n.$$

In the two examples we get 0.3405058416... and 0.3449916.... (if you use the definition given in the lecture notes instead of that given in the handout you will get 0.3449916... and 0.3461735...). The exact value is 0.34657359..., so the $n = 8$ result is closer.

The error term for the composite rule satisfies

$$|\text{error}| = \frac{h^2(b - a)}{6} |f''(\mu)| \leq \frac{h^2(b - a)}{6} \max_{a \leq x \leq b} |f''(x)|$$

for some $a \leq \mu \leq b$. In this case we have $a = 0, b = \pi/4$ and $f''(x) = 2 \tan x(1 + \tan^2 x)$. This is an increasing function of x and so the maximum value is at $x = \pi/4$ giving

$$|\text{error}| \leq \frac{h^2 \pi}{6 \times 4} |f''(\pi/4)| = \frac{h^2 \pi}{6}$$

where $h = \pi/(4n)$. The error bounds in the two cases are then $0.02 \dots$ and 0.005 and the actual errors (from above) are well within these bounds at 0.006 and 0.0016 .

To ensure that the error is $< 10^{-8}$ we need

$$\frac{h^2 \pi}{6} = \frac{\pi^3}{384n^2} < 10^{-8}.$$

Rearrange to pick out n^2

$$n^2 > \frac{10^8 \pi^3}{384} \Leftrightarrow n > 2841.575 \dots$$

so that the choosing $n \geq 2842$ guarantees that the error is small enough.

Question 8

Use the same process as for the Composite Simpson Rule in the notes. For the composite Trapezoidal Rule the total error over all n subintervals is

$$E = \sum_{j=1}^n \frac{-h^3}{12} f''(\zeta_j) = \frac{-h^3}{12} \sum_{j=1}^n f''(\zeta_j)$$

where $h = (b-a)/n$ and $x_{j-1} \leq \zeta_j \leq x_j$ (ζ_j is in the j th interval). Since each ζ_j lies in one of the subintervals between a and b , the value of $f''(\zeta_j)$ must be between the maximum and minimum that $f''(x)$ takes on the interval $[a, b]$. Hence:

$$\sum_{j=1}^n \min_{a \leq x \leq b} f''(x) \leq \sum_{j=1}^n f''(\zeta_j) \leq \sum_{j=1}^n \max_{a \leq x \leq b} f''(x)$$

and this simplifies to

$$n \min_{a \leq x \leq b} f''(x) \leq \sum_{j=1}^n f''(\zeta_j) \leq n \max_{a \leq x \leq b} f''(x).$$

Now if we say that the minimum occurs at $x = p$ and the maximum at $x = q$ and divide through by n we get:

$$f''(p) = \min_{a \leq x \leq b} f''(x) \leq \frac{1}{n} \sum_{j=1}^n f''(\zeta_j) \leq \max_{a \leq x \leq b} f''(x) = f''(q).$$

The Mean Value Theorem now lets us say that if $f''(x)$ is continuous (and we assume that it is), then

$$f''(p) \leq \frac{1}{n} \sum_{j=1}^n f''(\zeta_j) \leq f''(q) \Rightarrow \frac{1}{n} \sum_{j=1}^n f''(\zeta_j) = f''(\mu)$$

for some μ between p and q , which in turn lie between a, b . The result then follows:

$$E = \frac{-h^3}{12} \sum_{j=1}^n f''(\zeta_j) = \frac{-h^3}{12} n f''(\mu) = \frac{-h^2(b-a)}{12} f''(\mu)$$

since $nh = (b-a)$.