



- 1 Compute numerical approximations of the definite integral

$$\int_0^1 \sin(x^2) dx$$

using the composite trapezoid rule with $h = 1$, $h = 1/2$, and $h = 1/4$. In addition, provide estimates for the approximation error.

Possible solution:

The trapezoid rule yields the following approximations of the integral:

$$T(f, 0, 1) = \left(\frac{1}{2} \sin(0) + \frac{1}{2} \sin(1)\right) \approx 0.4207,$$

$$T(f, 0, 1, 1/2) = \frac{1}{2} \left(\frac{1}{2} \sin(0) + \sin(1/4) + \frac{1}{2} \sin(1)\right) \approx 0.3341,$$

$$T(f, 0, 1, 1/4) = \frac{1}{4} \left(\frac{1}{2} \sin(0) + \sin(1/16) + \sin(1/4) + \sin(9/16) + \frac{1}{2} \sin(1)\right) \approx 0.3160.$$

For the approximation error we use the estimate

$$|T(f, a, b, h) - \int_0^1 f(x) dx| \leq \frac{b-a}{12} h^2 \sup_{x \in [a,b]} |f''(x)|.$$

In our case,

$$f''(x) = 2 \cos(x^2) - 4x^2 \sin(x^2),$$

and thus (since \cos and \sin are both bounded by 1)

$$\sup_{x \in [0,1]} |f''(x)| \leq 6.$$

Hence we obtain

$$|T(f, a, b, h) - \int_0^1 f(x) dx| \leq \frac{h^2}{2}.$$

For $h = 1$, $h = 1/2$, and $h = 1/4$ the respective error bounds are therefore $1/2$, $1/8$, and $1/32$.¹

¹ In this case better estimates can be obtained quite easily: The function f'' is decreasing on the interval $[0, 1]$ because both $\cos(x^2)$ and $-x^2 \sin(x^2)$ are. Thus we can estimate

$$\sup_{x \in [0,1]} |f''(x)| \leq \max\{|f''(0)|, |f''(1)|\} \approx 2.285.$$

2 Compute numerical approximations of the definite integral

$$\int_0^2 e^{-x^2} \sin(x) dx$$

- a) using the composite trapezoid rule with $h = 1$ and $h = 1/2$,
 b) using the composite Simpson rule with $h = 1$ and $h = 1/2$,
 (You may want to use MATLAB for the computations.)

Possible solution:

a) For the trapezoid rule we obtain

$$T(f, 0, 2, 1) = \left(\frac{1}{2}f(0) + f(1) + \frac{1}{2}f(2) \right) \approx 0.3179.$$

and

$$T(f, 0, 2, 1/2) = \left(\frac{1}{2}f(0) + f(1/2) + f(1) + f(3/2) + \frac{1}{2}f(2) \right) \approx 0.3982.$$

b) The Simpson rule yields

$$S(f, 0, 2, 1) = \frac{1}{6}(f(0) + 4f(1/2) + 2f(1) + 4f(3/2) + f(2)) \approx 0.4250$$

and

$$S(f, 0, 2, 1/2) = \frac{1}{12}(f(0) + 4f(1/4) + 2f(1/2) + 4f(3/4) + 2f(1) + 4f(5/4) + 2f(3/2) + 4f(7/4) + f(2)) \approx 0.4213.$$

3 Compute numerical approximations of the definite integrals

$$\int_0^1 x^{7/2} dx \quad \text{and} \quad \int_0^1 x^{5/2} dx$$

using the trapezoid method and the Simpson method with $h = 1$, $h = 1/2$, $h = 1/4$.

- a) Compute for all approximations the respective approximation errors and try to estimate numerically the convergence rate.
 b) Which convergence rate would you usually expect for the trapezoid method and the Simpson method, and which have you actually observed? Try to explain possible discrepancies.

(You may want to use MATLAB for the computations.)

From this we would obtain the estimate

$$|T(f, a, b, h) - \int_0^1 f(x) dx| \leq \frac{2.285}{12} h^2$$

and hence the error estimates 0.1904, 0.0476, and 0.0119.

Possible solution:

The results of the numerical approximations with the trapezoid and the Simpson method are listed in the following table (all rounded to 7 significant digits):

$f(x) = x^{7/2}$:			$f(x) = x^{5/2}$:		
h	Trapezoid	Simpson	h	Trapezoid	Simpson
1	0.5	0.2255922	1	0.5	0.2845178
0.5	0.2941942	0.2224537	0.5	0.3383883	0.2855925
0.25	0.2403888	0.2222377	0.25	0.2987915	0.2857024

a) The exact values of the integrals are:

$$\int_0^1 x^{7/2} dx = \frac{2}{9} \approx 0.2222222,$$

$$\int_0^1 x^{5/2} dx = \frac{2}{7} \approx 0.2857143.$$

Thus we obtain the following approximate errors err_h :

$f(x) = x^{7/2}$:			$f(x) = x^{5/2}$:		
	Trapezoid	Simpson		Trapezoid	Simpson
err_1	0.2777778	0.0033701	err_1	0.2142857	0.0011965
$\text{err}_{0.5}$	0.0719720	0.0002315	$\text{err}_{0.5}$	0.0526741	0.0001217
$\text{err}_{0.25}$	0.0181666	0.0000154	$\text{err}_{0.25}$	0.0130772	0.0000118

In order to estimate the convergence rates, we compute next the ratios of consecutive approximations. For these we get

$f(x) = x^{7/2}$:			$f(x) = x^{5/2}$:		
	Trapezoid	Simpson		Trapezoid	Simpson
$\frac{\text{err}_1}{\text{err}_{0.5}}$	3.860	14.558	$\frac{\text{err}_1}{\text{err}_{0.5}}$	4.068	9.828
$\frac{\text{err}_{0.5}}{\text{err}_{0.25}}$	3.962	15.003	$\frac{\text{err}_{0.5}}{\text{err}_{0.25}}$	4.028	10.312

In case a method has approximation order $\mathcal{O}(h^p)$ for some $p > 0$, we would expect that

$$\frac{\text{err}_h}{\text{err}_{h/2}} \approx \frac{Ch^p}{C(h/2)^p} = 2^p.$$

Consequently, the number

$$\hat{p}_h := \log_2 \left(\frac{\text{err}_h}{\text{err}_{h/2}} \right)$$

should give us an estimate of the convergence order. We obtain

$f(x) = x^{7/2}$:			$f(x) = x^{5/2}$:		
	Trapezoid	Simpson		Trapezoid	Simpson
\hat{p}_1	1.949	3.864	\hat{p}_1	2.024	3.297
$\hat{p}_{0.5}$	1.986	3.907	$\hat{p}_{0.5}$	2.010	3.366

These results indicate that, most probably, the trapezoid rule has for both functions a convergence order of $\mathcal{O}(h^2)$. The convergence rates for the Simpson rule are not that easy to estimate. In case of the function $f(x) = x^{7/2}$ one can reasonably assume that the convergence order is $\mathcal{O}(h^4)$, although it would be also possible that it is slightly smaller; for the function $f(x) = x^{5/2}$, this convergence rate seems unlikely, and one would rather estimate a rate of $\mathcal{O}(h^{3.3})$ or $\mathcal{O}(h^{3.4})$.

- b) Usually, one would expect for the trapezoid method a convergence rate of $\mathcal{O}(h^2)$, and the computations confirm this expectation. The convergence rate for the Simpson method is usually $\mathcal{O}(h^4)$, but the numerical computations indicate that the rate is maybe not reached for the function $f(x) = x^{7/2}$ and almost surely not reached for the function $f(x) = x^{5/2}$. The problem is that the convergence rates result for the Simpson rule requires the function f to be four times differentiable. Both functions in this example, however, are not, and the second function is in fact only twice differentiable. (This is also the reasons why the trapezoid rule works just as expected.)

- 4 Derive the formula for the closed Newton–Cotes rule with $n = 4$ (with nodes $x_j = a + j(b - a)/4$, $0 \leq j \leq 4$).

Possible solution:

The weights for this Newton–Cotes rule have to satisfy the equations

$$\begin{aligned} 2 &= \int_{-1}^1 1 \, dx = 2(c_0 + c_1 + c_2 + c_3 + c_4), \\ 0 &= \int_{-1}^1 x \, dx = 2(-c_0 - \frac{1}{2}c_1 + \frac{1}{2}c_3 + c_4), \\ \frac{2}{3} &= \int_{-1}^1 x^2 \, dx = 2(c_0 + \frac{1}{4}c_1 + \frac{1}{4}c_3 + c_4), \\ 0 &= \int_{-1}^1 x^3 \, dx = 2(-c_0 - \frac{1}{8}c_1 + \frac{1}{8}c_3 + c_4), \\ \frac{2}{5} &= \int_{-1}^1 x^4 \, dx = 2(c_0 + \frac{1}{16}c_1 + \frac{1}{16}c_3 + c_4). \end{aligned}$$

From the second and the fourth equation (or the symmetry of the nodes) we obtain that $c_0 = c_4$ and $c_1 = c_3$. Thus the third and the fifth equation simplify to

$$\begin{aligned} \frac{1}{3} &= 2c_0 + \frac{1}{2}c_1, \\ \frac{1}{5} &= 2c_0 + \frac{1}{8}c_1. \end{aligned}$$

From this we immediately obtain that

$$c_1 = c_3 = \frac{16}{45}$$

and thus

$$c_0 = c_4 = \frac{1}{6} - \frac{1}{4}c_1 = \frac{7}{90}.$$

Finally,

$$c_2 = 1 - c_0 - c_1 - c_3 - c_4 = \frac{2}{15}.$$

Thus the closed Newton–Cotes rule with $n = 4$

$$Q(f, a, b) = (b - a) \left(\frac{7}{90}f(y_0) + \frac{16}{45}f(y_1) + \frac{2}{15}f(y_2) + \frac{16}{45}f(y_3) + \frac{7}{90}f(y_4) \right).$$

5 Construct for every $0 < \alpha < 1$ a quadrature rule of the form

$$Q(f, -1, 1) = 2(c_0f(-\alpha) + c_1f(0) + c_2f(\alpha))$$

that has degree of precision 2, i.e. integrates all polynomials up to degree 2 exactly.

It might be possible that polynomials of higher order than 2 are integrated exactly.

What is the actual degree of precision of the different formulas?

Possible solution:

The rule has to satisfy the equations

$$\begin{aligned} 2 &= \int_{-1}^1 1 \, dx = 2(c_0 + c_1 + c_2), \\ 0 &= \int_{-1}^1 x \, dx = 2(-\alpha c_0 + \alpha c_2), \\ \frac{2}{3} &= \int_{-1}^1 x^2 \, dx = 2(\alpha^2 c_0 + \alpha^2 c_2). \end{aligned}$$

The second equation implies that $c_0 = c_2$; the third equation implies

$$c_0 = c_2 = \frac{1}{6\alpha^2}.$$

The first equation now implies that

$$c_1 = 1 - \frac{1}{3\alpha^2} = \frac{3\alpha^2 - 1}{3\alpha^2}.$$

For finding the actual degree of precision, we check whether also polynomials of higher degree are integrated exactly. We note first that

$$Q(x^3, -1, 1) = 2 \left(-\frac{1}{6\alpha^2}\alpha^3 + 0 + \frac{1}{6\alpha^2}\alpha^3 \right) = 0 \int_{-1}^1 x^3 \, dx,$$

which shows that the (composite) rules have degree of precision at least 3. Next we note that

$$\int_{-1}^1 x^4 \, dx = \frac{2}{5}$$

and

$$Q(x^4, -1, 1) = 2\left(\frac{1}{6\alpha^2}\alpha^4 + \frac{1}{6\alpha^2}\alpha^4\right) = \frac{2}{3}\alpha^2.$$

Thus the function x^4 is integrated exactly, if and only if $\alpha^2 = 3/5$ or

$$\alpha = \sqrt{\frac{3}{5}}.$$

Thus the degree of precision for $\alpha^2 \neq 3/5$ is 3. For the case $\alpha^2 = 3/5$

$$Q(x^5, -1, 1) = 2\left(-\frac{1}{6\alpha^2}\alpha^5 + \frac{1}{6\alpha^2}\alpha^5\right) = 0 = \int_{-1}^1 x^5 dx,$$

but

$$Q(x^6, -1, 1) = 2\left(\frac{1}{6\alpha^2}\alpha^6 + \frac{1}{6\alpha^2}\alpha^6\right) = \frac{2}{3}\alpha^4 = \frac{2}{3} \frac{9}{25} = \frac{6}{25}$$

and

$$\int_{-1}^1 x^6 dx = \frac{2}{7}.$$

This shows that the degree of precision for $\alpha^2 = 3/5$ is 5.

To summarize, we have a degree of precision 3 for $\alpha^2 \neq 3/5$, and 5 for $\alpha^2 = 3/5$.

- 6 Implement and use Romberg integration to approximate the integrals in Exercise 2. Compute the Romberg table until either $|R_{n-1,n-1} - R_{n,n}| < 10^{-6}$. Compare your result to the exact value of the integral.

Possible solution:

A function that computes the Romberg Array in MATLAB is implemented in the function `romint`.

For the integral $\int_0^2 e^{-x^2} \sin(x) dx$ the algorithm converges for $n = 6$ to the approximation $R(6, 6) = 0.4211642$. This matches the true solution to the digits given. The actual error is 1.67×10^{-12} , well below 10^{-6} .

- 7 Romberg integration is used to approximate $\int_2^3 f(x) dx$. If $f(2) = 0.51342$, $f(3) = 0.36788$, $R(2, 0) = 0.43687$, and $R(2, 2) = 0.43662$, find $f(2.5)$.

Possible solution:

We have $b - a = 1$ and can thus compute $R(0, 0)$ since

$$R(0, 0) = \frac{1}{2}(f(2) + f(3)) = 0.44065.$$

In addition

$$R(1, 0) = \frac{1}{2}(R(0, 0) + f(2.5)).$$

From the Richardson extrapolation formula and the above relation

$$\begin{aligned}R(1, 1) &= \frac{4}{3}R(1, 0) - \frac{1}{3}R(0, 0) = \frac{1}{3}R(0, 0) + \frac{2}{3}f(2.5) \\R(2, 1) &= \frac{4}{3}R(2, 0) - \frac{1}{3}R(1, 0) = \frac{4}{3}R(2, 0) - \frac{1}{6}R(0, 0) - \frac{1}{6}f(2.5) \\R(2, 2) &= \frac{16}{15}R(2, 1) - \frac{1}{15}R(1, 1) \\&= \frac{16}{15} \left(\frac{4}{3}R(2, 0) - \frac{1}{6}R(0, 0) - \frac{1}{6}f(2.5) \right) - \frac{1}{15} \left(\frac{1}{3}R(0, 0) + \frac{2}{3}f(2.5) \right) \\&= \frac{64}{45}R(2, 0) - \frac{1}{5}R(0, 0) - \frac{2}{9}f(2.5)\end{aligned}$$

Isolating $f(2.5)$ in the last equation yields

$$f(2.5) = \frac{64R(2, 0) - 9R(0, 0) - 45R(2, 2)}{10} \approx 0.43459$$