7

Numerical integration – I

7.1 Introduction

The problem of evaluating definite integrals arises both in mathematics and beyond, in many areas of science and engineering. At some point in our mathematical education we all learned to calculate simple integrals such as

$$\int_0^1 \mathrm{e}^x \mathrm{d}x \qquad \text{or} \qquad \int_0^\pi \cos x \, \mathrm{d}x$$

using a table of integrals, so you will know that the values of these are $\mathrm{e} - 1$ and 0 respectively; but how about the innocent-looking

$$\int_0^1 \mathrm{e}^{x^2} \mathrm{d}x \qquad \text{and} \qquad \int_0^\pi \cos(x^2) \mathrm{d}x \,,$$

or the more exotic

$$\int_1^{2000} \exp(\sin(\cos(\sinh(\cosh(\tan^{-1}(\log(x))))))) \, \mathrm{d}x?$$

Please try to evaluate these using a table of integrals and see how far you can get! It is not so simple, is it? Of course, you could argue that the last example was completely artificial. Still, it illustrates the point that it is relatively easy to think of a continuous real-valued function f defined on a closed interval $[a, b]$ of the real line such that the definite integral

$$\int_a^b f(x) \, \mathrm{d}x \tag{7.1}$$

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is very hard to reduce to an entry in the table of integrals by means of the usual tricks of variable substitution and integration by parts. If you have access to the computer package Maple, you may try to type

```
evalf(int(exp(sin(cos(sinh(cosh(arctan(log(x))))))), x=1..2000));
```

at the Maple command line. In about the same time as it will take you to correctly type the command at the keyboard, as if by magic, the result 1514.780678 will pop up on the screen. How was this number arrived at?

The purpose of this chapter, and its continuation, Chapter 10, is to answer this question. Specifically, we shall address the problem of evaluating (7.1) approximately, by applying the results of Chapter 6 on polynomial interpolation to derive formulae for numerical integration (also called numerical quadrature rules). We shall also explain how one can estimate the associated approximation error. What does polynomial interpolation have to do with evaluating definite integrals? The answer will be revealed in the next section which is about a class of quadrature formulae bearing the names of two English mathematicians: Newton and Cotes.[1]

7.2 Newton–Cotes formulae

Let f be a real-valued function, defined and continuous on the closed real interval $[a, b]$, and suppose that we have to evaluate the integral

$$\int_a^b f(x)\mathrm{d}x\,.$$

Since polynomials are easy to integrate, the idea, roughly speaking, is to approximate the function f by its Lagrange interpolation polynomial p_n of degree n, and integrate p_n instead. Thus,

$$\int_a^b f(x)\mathrm{d}x \approx \int_a^b p_n(x)\mathrm{d}x\,. \tag{7.2}$$

For a positive integer n, let $x_i,\ i = 0, 1, \ldots, n$, denote the interpolation

[1] Roger Cotes (10 July 1682, Burbage, Leicestershire, England – 5 June 1716, Cambridge, Cambridgeshire, England) was a fellow of Trinity College in Cambridge. At the age of 26 he became the first Plumian Professor of Astronomy and Experimental Philosophy. Even though he only published one paper in his lifetime, entitled 'Logometria', Cotes made important contributions to the theory of logarithms and integral calculus, particularly interpolation and table construction. In reference to Cotes' early death, Newton said: *If he had lived we might have known something.*

points; for the sake of simplicity, we shall assume that these are equally spaced, that is,

$$x_i = a + ih\,, \qquad i = 0, 1, \ldots, n\,,$$

where

$$h = (b-a)/n\,.$$

The Lagrange interpolation polynomial of degree n for the function f, with these interpolation points, is of the form

$$p_n(x) = \sum_{k=0}^{n} L_k(x) f(x_k) \quad \text{where} \quad L_k(x) = \prod_{\substack{i=0\\ i\neq k}}^{n} \frac{x - x_i}{x_k - x_i}\,.$$

Inserting the expression for p_n into the right-hand side of (7.2) yields

$$\int_a^b f(x)\mathrm{d}x \approx \sum_{k=0}^{n} w_k f(x_k)\,, \tag{7.3}$$

where

$$w_k = \int_a^b L_k(x)\mathrm{d}x\,, \qquad k = 0, 1, \ldots, n\,. \tag{7.4}$$

The values w_k, $k = 0, 1, \ldots, n$, are referred to as the **quadrature weights**, while the interpolation points x_k, $k = 0, 1, \ldots, n$, are called the **quadrature points**. The numerical quadrature rule (7.3), with quadrature weights (7.4) and equally spaced quadrature points, is called the **Newton–Cotes formula** of order n. In order to illustrate the general idea, we consider two simple examples.

Trapezium rule. In this case we take $n = 1$, so that $x_0 = a$, $x_1 = b$; the Lagrange interpolation polynomial of degree 1 for the function f is simply

$$\begin{aligned} p_1(x) &= L_0(x)f(a) + L_1(x)f(b) \\ &= \frac{x-b}{a-b} f(a) + \frac{x-a}{b-a} f(b) \\ &= \frac{1}{b-a}[(b-x)f(a) + (x-a)f(b)]\,. \end{aligned}$$

Integrating $p_1(x)$ from a to b yields

$$\int_a^b f(x)\mathrm{d}x \approx \frac{b-a}{2}[f(a) + f(b)]\,.$$

This numerical integration formula is called the trapezium rule. The

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terminology stems from the fact that the expression on the right is the area of the trapezium with vertices $(a, 0)$, $(b, 0)$, $(a, f(a))$, $(b, f(b))$.

Simpson's rule.[1] A slightly more sophisticated quadrature rule is obtained by taking $n = 2$. In this case $x_0 = a$, $x_1 = (a + b)/2$ and $x_2 = b$, and the function f is approximated by a quadratic Lagrange interpolation polynomial.

The quadrature weights are calculated from

$$\begin{aligned} w_0 &= \int_a^b L_0(x)\mathrm{d}x \\ &= \int_a^b \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}\mathrm{d}x \\ &= \int_{-1}^1 \frac{t(t-1)}{2}\,\frac{b-a}{2}\mathrm{d}t \\ &= \frac{b-a}{6}, \end{aligned}$$

where it is convenient to make the change of variable

$$x = \frac{b-a}{2}\,t + \frac{b+a}{2}\,.$$

Similarly, $w_1 = \frac{4}{6}(b-a)$, and it is easy to see that $w_2 = w_0$ by symmetry. This gives

$$\int_a^b f(x)\mathrm{d}x \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right],$$

a numerical integration formula known as Simpson's rule.

It is very important to notice that the weights w_k defined in (7.4) depend only on n and k, not on the function f. Their values can therefore

[1] Thomas Simpson (20 August 1710, Market Bosworth, Leicestershire, England – 14 May 1761, Market Bosworth, Leicestershire, England) was a weaver by training who taught mathematics in the London coffee-houses. His two-volume work entitled *The Doctrine and Application of Fluxions* published in 1750 contains some of the work that Cotes hoped to publish with Cambridge University Press but was prevented by his premature death. In 1796 fellow mathematician Charles Hutton gave the following description of Simpson: *It has been said that Mr Simpson frequented low company, with whom he used to guzzle porter and gin: but it must be observed that the misconduct of his family put it out of his power to keep the company of gentlemen, as well as to procure better liquor.* On a related subject: in his *New Stereometry of Wine Barrels* (*Nova stereometria doliorum vinariorum* (1615)), the astronomer Johannes Kepler (1571–1630) approximated the volumes of many three-dimensional solids, each of which was formed by revolving a two-dimensional region around an axis line. For each of these volumes of revolution, he subdivided the solid into many thin slices the sum of whose volumes then approximated the desired total volume.

be calculated in advance, as in the trapezium rule and Simpson's rule. The evaluation of the approximation to the integral (7.1) is then a trivial matter; it is only necessary to compute $f(x_k)$ at each of the quadrature points x_k, $k = 0, 1, \ldots, n$, multiply by the known weights w_k for $k = 0, 1, \ldots, n$, and form the sum on the right-hand side of (7.3).

7.3 Error estimates

Our next task is to estimate the size of the error in the numerical integration formula (7.3), that is, the error that has been committed by integrating the interpolating Lagrange polynomial of f instead of f itself. The error in (7.3) is defined by

$$E_n(f) = \int_a^b f(x)\mathrm{d}x - \sum_{k=0}^{n} w_k f(x_k)\,.$$

The next theorem provides a useful bound on $E_n(f)$ under the additional hypothesis that the function f is sufficiently smooth.

Theorem 7.1 *Let $n \geq 1$. Suppose that f is a real-valued function, defined and continuous on the interval $[a, b]$, and let $f^{(n+1)}$ be defined and continuous on $[a, b]$. Then,*

$$|E_n(f)| \leq \frac{M_{n+1}}{(n+1)!} \int_a^b |\pi_{n+1}(x)|\,\mathrm{d}x\,, \tag{7.5}$$

where $M_{n+1} = \max_{\zeta\in[a,b]} |f^{(n+1)}(\zeta)|$ and $\pi_{n+1}(x) = (x-x_0)\ldots(x-x_n)$.

Proof Recalling the definition of the weights w_k from (7.4), we can write $E_n(f)$ as follows:

$$\begin{aligned} E_n(f) &= \int_a^b f(x)\,\mathrm{d}x - \int_a^b \left(\sum_{k=0}^{n} L_k(x) f(x_k)\right) \mathrm{d}x \\ &= \int_a^b [f(x) - p_n(x)]\,\mathrm{d}x\,. \end{aligned}$$

Thus,

$$|E_n(f)| \leq \int_a^b |f(x) - p_n(x)|\,\mathrm{d}x\,.$$

The desired error estimate (7.5) follows by inserting (6.8) into the right-hand side of this inequality. □

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Let us use this theorem to estimate the size of the error which arises from applying the trapezium rule to the integral $\int_a^b f(x)\,\mathrm{d}x$. In this case, with $n = 1$ and $\pi_2(x) = (x-a)(x-b)$, the bound (7.5) reduces to

$$\begin{aligned} |E_1(f)| &\le \frac{M_2}{2}\int_a^b |(x-a)(x-b)|\,\mathrm{d}x \\ &= \frac{M_2}{2}\int_a^b (b-x)(x-a)\,\mathrm{d}x \\ &= \frac{(b-a)^3}{12}M_2\,. \end{aligned} \tag{7.6}$$

An analogous but slightly more tedious calculation shows that, for Simpson's rule,

$$\begin{aligned} |E_2(f)| &\le \frac{M_3}{6}\int_a^b |(x-a)(x-(a+b)/2)(x-b)|\,\mathrm{d}x \\ &= \frac{(b-a)^4}{196}M_3\,. \end{aligned} \tag{7.7}$$

Unfortunately, (7.7) gives a considerable overestimate of the error in Simpson's rule; in particular it does not bring out the fact that $E_2(f) = 0$ whenever f is a polynomial of degree 3. The next theorem will allow us to give a sharper bound on the error in Simpson's rule which illustrates this fact. More generally, it is quite easy to prove that when n is odd the Newton–Cotes formula (7.3) (with w_k defined by (7.4)) is exact for all polynomials of degree n, while when n is even it is also exact for all polynomials of degree $n+1$ (see Exercise 2 at the end of the chapter).

Theorem 7.2 *Suppose that f is a real-valued function, defined and continuous on the interval $[a,b]$, and that $f^{\mathrm{iv}} = f^{(4)}$, the fourth derivate of f, is continuous on $[a,b]$. Then,*

$$\int_a^b f(x)\,\mathrm{d}x - \frac{b-a}{6}\,[f(a) + 4f((a+b)/2) + f(b)] = -\frac{(b-a)^5}{2880}f^{\mathrm{iv}}(\xi)\,, \tag{7.8}$$

for some ξ in (a,b).

Proof Making the change of variable

$$x = \frac{a+b}{2} + \frac{b-a}{2}t\,, \qquad t \in [-1,1]\,,$$

and defining the function $t \mapsto F(t)$ by $F(t) = f(x)$, we see that

$$\int_a^b f(x)\mathrm{d}x - \frac{b-a}{6}\left[f(a) + 4f((a+b)/2) + f(b)\right]$$
$$= \frac{b-a}{2}\left(\int_{-1}^{1} F(\tau)\mathrm{d}\tau - \frac{1}{3}[F(-1) + 4F(0) + F(1)]\right). \quad (7.9)$$

We now introduce the function $t \mapsto G(t)$ by

$$G(t) = \int_{-t}^{t} F(\tau)\,\mathrm{d}\tau - \frac{t}{3}[F(-t) + 4F(0) + F(t)]\,, \qquad t \in [-1,1]\,;$$

the right-hand side of (7.9) is then simply $\frac{1}{2}(b-a)G(1)$.

The remainder of the proof is devoted to showing that $\frac{1}{2}(b-a)G(1)$ is, in turn, equal to the right-hand side of (7.8) for some ξ in (a,b). To do so, we define

$$H(t) = G(t) - t^5 G(1)\,, \qquad t \in [-1,1]\,,$$

and apply Rolle's Theorem repeatedly to the function H. Noting that $H(0) = H(1) = 0$, we deduce that there exists $\zeta_1 \in (0,1)$ such that $H'(\zeta_1) = 0$. But it is easy to show that $H'(0) = 0$, so there exists $\zeta_2 \in (0,\zeta_1)$ such that $H''(\zeta_2) = 0$. Again we see that $H''(0) = 0$, so there exists $\zeta_3 \in (0,\zeta_2)$ such that $H'''(\zeta_3) = 0$. Now,

$$G'''(t) = -\frac{t}{3}[F'''(t) - F'''(-t)]\,,$$

and therefore

$$H'''(\zeta_3) = -\frac{\zeta_3}{3}[F'''(\zeta_3) - F'''(-\zeta_3)] - 60\zeta_3^2 G(1)\,.$$

Applying the Mean Value Theorem to the function F''' this shows that there exists $\zeta_4 \in (-\zeta_3,\zeta_3)$ such that

$$\begin{aligned} H'''(\zeta_3) &= -\frac{\zeta_3}{3}[2\zeta_3 F^{\mathsf{iv}}(\zeta_4)] - 60\zeta_3^2 G(1) \\ &= -\frac{2\zeta_3^2}{3}[F^{\mathsf{iv}}(\zeta_4) + 90G(1)]\,. \end{aligned}$$

Since $H'''(\zeta_3) = 0$ and $\zeta_3 \neq 0$, this means that

$$G(1) = -\frac{1}{90}F^{\mathsf{iv}}(\zeta_4) = -\frac{(b-a)^4}{1440}f^{\mathsf{iv}}(\xi)\,,$$

and the required result follows. □

Theorem 7.2 yields the following bound on the error in Simpson's rule:

$$|E_2(f)| \le \frac{(b-a)^5}{2880} M_4 \,. \tag{7.10}$$

This is a considerable improvement on the earlier bound (7.7); when f is a polynomial of degree 3, the bound correctly shows that $E_2(f) = 0$.

There is a great variety of quadrature rules constructed in the same way as the Newton–Cotes formulae. For example, it may sometimes be useful to involve quadrature points outside the interval of integration, as in

$$\int_0^1 f(x)\,\mathrm{d}x \approx c_{-1} f(-1) + c_0 f(0) + c_1 f(1)\,. \tag{7.11}$$

The coefficients are determined similarly as in (7.4), but now $x_{-1} = -1$, $x_0 = 0$, $x_1 = 1$ and

$$L_{-1}(x) = \tfrac{1}{2}x(x-1)\,, \quad L_0(x) = 1 - x^2\,, \quad L_1(x) = \tfrac{1}{2}x(x+1)\,.$$

Hence,

$$\begin{aligned} c_{-1} &= \int_0^1 L_{-1}(x)\,\mathrm{d}x \\ &= \int_0^1 \frac{x(x-1)}{2}\,\mathrm{d}x \\ &= -\tfrac{1}{12}\,. \end{aligned}$$

In a similar way we find that $c_0 = \frac{2}{3}$, $c_1 = \frac{5}{12}$.

The quadrature rule (7.11) is then exact when f is any polynomial of degree 2 or less. More generally, for any three times continuously differentiable function f, Theorem 7.1 extends in an obvious way to give

$$\begin{aligned} &\left| \int_0^1 f(x)\,\mathrm{d}x + \tfrac{1}{12} f(-1) - \tfrac{2}{3} f(0) - \tfrac{5}{12} f(1) \right| \\ &\qquad\qquad \le \frac{M_3}{6} \int_0^1 |(x+1)x(x-1)|\,\mathrm{d}x \\ &\qquad\qquad \le \frac{M_3}{24}\,; \end{aligned}$$

but there is an important difference. To justify this estimate we now need a condition on f outside the interval of integration: we must require that f and f''' are continuous on $[-1, 1]$, and M_3 is the maximum of $|f'''(x)|$ on $[-1, 1]$. More generally, the conditions must hold on an interval which contains the interval of integration, and also all the quadrature points.

Table 7.1. *I_n is the result of the Newton–Cotes formula of degree n for the approximation of the integral (7.12)*

n	I_n
1	0.38462
2	6.79487
3	2.08145
4	2.37401
5	2.30769
6	3.87045
7	2.89899
8	1.50049
9	2.39862
10	4.67330
11	3.24477
12	−0.31294
13	1.91980
14	7.89954
15	4.15556

7.4 The Runge phenomenon revisited

By looking at the right-hand side of the error bound (7.5) we may be led to believe that by increasing n, that is by approximating the integrand by Lagrange interpolation polynomials of increasing degree and integrating these exactly, we shall reduce the size of the quadrature error $E_n(f)$. However, this is not always the case, even for very smooth functions f. An example of this behaviour uses the same function as in Section 6.3; Table 7.1 gives the results of applying Newton–Cotes formulae of increasing degree to the evaluation of the integral

$$\int_{-5}^{5} \frac{1}{1+x^2}\,\mathrm{d}x\,. \tag{7.12}$$

These results do not evidently converge as n increases, and in fact they eventually increase without bound. This behaviour is related to the fact that the weights w_j in the Newton–Cotes formula are not all positive when $n > 8$. We shall return to this point in Theorem 10.2.

A better approach to improving accuracy is to divide the interval $[a, b]$ into an increasing number of subintervals of decreasing size, and then to use a numerical integration formula of fixed order n on each of the subintervals. Quadrature rules based on this approach are called composite formulae; in the next section we shall describe two examples.[1]

7.5 Composite formulae

We shall consider only some very simple composite quadrature rules: the composite trapezium rule and the composite Simpson rule.

Suppose that f is a function, defined and continuous on a nonempty closed interval $[a,b]$ of the real line. In order to construct an approximation to

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

we now select an integer $m \geq 2$ and divide the interval $[a,b]$ into m equal subintervals, each of width $h = (b-a)/m$, so that

$$\int_a^b f(x)\,\mathrm{d}x = \sum_{i=1}^{m} \int_{x_{i-1}}^{x_i} f(x)\,\mathrm{d}x\,, \tag{7.13}$$

where

$$x_i = a + ih = a + \frac{i}{m}(b-a)\,, \quad i = 0,1,\ldots,m\,.$$

Each of the integrals is then evaluated by the trapezium rule,

$$\int_{x_{i-1}}^{x_i} f(x)\,\mathrm{d}x \approx \frac{1}{2}h[f(x_{i-1}) + f(x_i)]\,; \tag{7.14}$$

summing these over $i = 1, 2, \ldots, m$ leads to the following definition.

Definition 7.1 (Composite trapezium rule)

$$\boxed{\int_a^b f(x)\,\mathrm{d}x \approx h\left[\frac{1}{2}f(x_0) + f(x_1) + \cdots + f(x_{m-1}) + \frac{1}{2}f(x_m)\right]. \quad (7.15)}$$

[1] The historical roots of composite formulae may be traced back to the work of Kepler cited in the footnote to Simpson's method earlier on in this chapter, although the idea of computing volumes of two- and three-dimensional geometrical objects by subdivision was already present in the work of Archimedes of Syracuse (287 BC, Syracuse (now in Italy) – 212 BC, Syracuse (now in Italy)). Archimedes' long-lost book known as the Palimpsest, containing his geometrical studies, resurfaced at an auction at Christie's of New York in 1998 and is now in the care of the Walters Art Gallery in Baltimore, Maryland, USA: `http://www.thewalters.org/archimedes/frame.html`

The error in the composite trapezium rule can be estimated by using the error bound (7.6) for the trapezium rule on each individual subinterval $[x_{i-1}, x_i]$, $i = 1, 2, \dots, m$. For this purpose, let us define

$$\begin{aligned}
\mathcal{E}_1(f) &= \int_a^b f(x)\,\mathrm{d}x - h\left[\tfrac{1}{2}f(x_0) + f(x_1) + \cdots + f(x_{m-1}) + \tfrac{1}{2}f(x_m)\right] \\
&= \sum_{i=1}^{m}\left[\int_{x_{i-1}}^{x_i} f(x)\,\mathrm{d}x - \tfrac{1}{2}h\left[f(x_{i-1}) + f(x_i)\right]\right].
\end{aligned}$$

Applying (7.6) to each of the terms under the summation sign we obtain

$$\begin{aligned}
|\mathcal{E}_1(f)| &\le \frac{1}{12}h^3\sum_{i=1}^{m}\left(\max_{\zeta\in[x_{i-1},x_i]}|f''(\zeta)|\right) \\
&\le \frac{(b-a)^3}{12m^2}M_2\,, \qquad (7.16)
\end{aligned}$$

where $M_2 = \max_{\zeta\in[a,b]}|f''(\zeta)|$.

For Simpson's rule, let us suppose that the interval $[a, b]$ has been divided into $2m$ intervals by the points $x_i = a + ih$, $i = 0, 1, \dots, 2m$, with $m \ge 2$ and

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

and let us apply Simpson's rule on each of the intervals $[x_{2i-2}, x_{2i}]$, $i = 1, 2, \dots, m$, giving

$$\begin{aligned}
\int_a^b f(x)\,\mathrm{d}x &= \sum_{i=1}^{m}\int_{x_{2i-2}}^{x_{2i}} f(x)\,\mathrm{d}x \\
&\approx \sum_{i=1}^{m}\frac{2h}{6}\left[f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})\right].
\end{aligned}$$

This leads to the following definition.

Definition 7.2 (Composite Simpson rule)

$$\begin{aligned}
\int_a^b f(x)\,\mathrm{d}x \approx{}& \frac{h}{3}\left[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \cdots\right. \\
&\left.+ 2f(x_{2m-2}) + 4f(x_{2m-1}) + f(x_{2m})\right]. \qquad (7.17)
\end{aligned}$$

A schematic view of the pattern in which the coefficients 1, 4 and 2 appear in the composite Simpson rule is shown in Figure 7.1.

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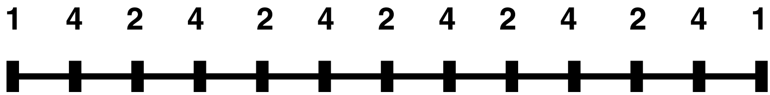

Fig. 7.1. Quadrature weights for the composite Simpson rule: the integers $1, 4, 2, 4, \ldots, 1$, when multiplied by $h/3$, where $h = (b-a)/2m$, provide the quadrature weights. This figure corresponds to taking $m = 6$.

In order to estimate the error in the composite Simpson rule, we proceed in the same way as for the composite trapezium rule. Let us define

$$\begin{aligned}\mathcal{E}_2(f) &= \int_a^b f(x)\,\mathrm{d}x - \sum_{i=1}^{m} \frac{h}{3}[f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})] \\ &= \sum_{i=1}^{m} \left[\int_{x_{2i-2}}^{x_{2i}} f(x)\,\mathrm{d}x - \frac{h}{3}[f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})]\right].\end{aligned}$$

Applying (7.10) to each individual term in the sum and recalling that $b - a = 2mh$ we obtain the following error bound:

$$|\mathcal{E}_2(f)| \le \frac{(b-a)^5}{2880m^4} M_4\,, \tag{7.18}$$

where $M_4 = \max_{\zeta\in[a,b]} |f^{iv}(\zeta)|$.

The composite rules (7.15) and (7.17) provide greater accuracy than the basic formulae considered in Section 7.2; this is clearly seen by comparing the error bounds (7.16) and (7.18) for the two composite rules with (7.6) and (7.8), the error estimates for the basic trapezium rule and Simpson rule respectively. The inequalities (7.16) and (7.18) indicate that, as long as the function f is sufficiently smooth, the errors in the composite rules can be made arbitrarily small by choosing a sufficiently large number of subintervals.

7.6 The Euler–Maclaurin expansion

We have seen in (7.16) that the error in the composite trapezium rule is bounded by a term involving $1/m^2$, where m is the number of subdivisions of the interval $[a, b]$; the **Euler**[1]–**Maclaurin**[2] expansion expresses this error as a series in powers of $1/m^2$, and makes it possible to improve accuracy by extrapolation methods.

We first define a sequence of polynomials.

Definition 7.3 *Consider the sequence of polynomials q_r, $r = 1, 2, \ldots$, defined by their properties, as follows:*

(i) *q_r is a polynomial of degree r;*
(ii) *for each positive integer r, $q'_{r+1} = q_r$;*
(iii) *q_r is an odd function if r is odd, and an even function if r is even;*
(iv) *if $r > 1$ is odd, then $q_r(-1) = 0$ and $q_r(1) = 0$;*
(v) *$q_1(t) = -t$.*

Using these conditions it is easy to construct the polynomials q_r in succession. From (v) and (ii) we get

$$q_2(t) = -\tfrac{1}{2}t^2 + A_2\,, \qquad q_3(t) = -\tfrac{1}{6}t^3 + A_2 t + A_3\,,$$

where A_2 and A_3 are constants. From (iii) we see that $A_3 = 0$; then, from (iv) it follows that $A_2 = \frac{1}{6}$. Hence,

$$q_2(t) = -\tfrac{1}{2}t^2 + \tfrac{1}{6}\,, \qquad q_3(t) = -\tfrac{1}{6}t^3 + \tfrac{1}{6}t\,.$$

We can then go on to construct q_4 and q_5, and so on.

[1] Leonhard Euler (15 April 1707, Basel, Switzerland – 18 September 1783, St Petersburg, Russia) was the most prolific mathematical writer of all times, who made fundamental contributions to many branches of mathematics despite being totally blind for the last third of his life. Euler and his wife Katharina had 13 children: he claimed to have made his greatest discoveries while he was holding a baby in his arms and the other children were playing around his feet. Euler studied the calculus of variations, differential geometry, number theory, differential equations, continuum mechanics, astronomy, lunar theory, the three-body problem, elasticity, acoustics, the wave theory of light, hydraulics, and music. In his *Theory of the Motions of Rigid Bodies* published in 1765 he laid the foundation of analytical mechanics. Euler integrated Leibniz's differential calculus and Newton's method of fluxions into mathematical analysis. We owe him the concepts of beta and gamma functions and the notion of integrating factor for differential equations; he is responsible for the notation e for the base of natural logarithm, $f(x)$ for a function, π for pi, $\sum$ for summation, i for the square root of -1, and Δ_y and Δ_y^2 for the first and second finite differences.

[2] Colin Maclaurin (February 1698, Kilmodan, Argyllshire, Scotland – 14 June 1746, Edinburgh, Scotland) became a student at the University of Glasgow at the age of 11 and completed his studies at the age of 14. In 1719, at the age of 21, he became Fellow of the Royal Society. His major work of 763 pages in two volumes, entitled *A Treatise of Fluxions*, was the first systematic exposition of Newton's ideas. Notable is Maclaurin's work on elliptic integrals, maxima and minima, and the attraction of ellipsoids.

Theorem 7.3 *Suppose that the function g is defined and continuous on the interval $[-1,1]$ and has a continuous derivative of order $2k$ over this interval. Then,*

$$\int_{-1}^{1} g(t)\,\mathrm{d}t - [g(-1)+g(1)] = \int_{-1}^{1} -t\,g'(t)\,\mathrm{d}t$$
$$= \sum_{r=1}^{k} q_{2r}(1)[g^{(2r-1)}(1) - g^{(2r-1)}(-1)] - \int_{-1}^{1} q_{2k}(t)g^{(2k)}(t)\,\mathrm{d}t\,. \quad (7.19)$$

Proof We observe that $\int_{-1}^{1} g(t)\,\mathrm{d}t - [g(-1)+g(1)]$ is the error in the approximation of $\int_{-1}^{1} g(t)\mathrm{d}t$ by the trapezium rule. Integration by parts gives

$$\int_{-1}^{1} -t\,g'(t)\,\mathrm{d}t \quad = \quad -[g(-1)+g(1)] + \int_{-1}^{1} g(t)\,\mathrm{d}t\,,$$

which establishes the first equality in (7.19). By repeated integration by parts in the other direction, and using the fact that $q_1(t) = -t$, we then have

$$\begin{aligned}\int_{-1}^{1} -t\,g'(t)\,\mathrm{d}t &= q_2(1)g'(1) - q_2(-1)g'(-1) - \int_{-1}^{1} q_2(t)g''(t)\mathrm{d}t \\ &= \Big[q_2(t)g'(t) - q_3(t)g''(t) + \cdots + q_{2k}(t)g^{(2k-1)}(t)\Big]_{-1}^{1} \\ &\quad - \int_{-1}^{1} q_{2k}(t)g^{(2k)}(t)\,\mathrm{d}t\,.\end{aligned}$$

The required result follows from properties (iii) and (iv) of the q_r. □

Theorem 7.4 (Euler–Maclaurin expansion) *Suppose that the real-valued function f is defined and continuous on the interval $[a,b]$ and has a continuous derivative of order $2k$ on this interval. Consider the subdivision of $[a,b]$ into $m \geq 1$ closed intervals $[x_{i-1}, x_i]$, $i = 1,\ldots,m$, where $x_i = a + ih$, $i = 0,1,\ldots,m$, and $h = (b-a)/m$. Writing $T(m)$ for the result of approximating the integral $I = \int_a^b f(x)\mathrm{d}x$ by the composite trapezium rule with the m subintervals $[x_{i-1}, x_i]$, $i = 1,\ldots,m$,*

$$\begin{aligned}I - T(m) &= \sum_{r=1}^{k} c_r h^{2r}[f^{(2r-1)}(b) - f^{(2r-1)}(a)] \\ &\quad - \left(\frac{h}{2}\right)^{2k} \sum_{i=1}^{m} \int_{x_{i-1}}^{x_i} q_{2k}(t) f^{(2k)}(x)\,\mathrm{d}x\,, \qquad (7.20)\end{aligned}$$

where $t = t(x) = -1 + \frac{2}{h}(x - x_{i-1})$ for $x \in [x_{i-1}, x_i]$, $i = 1, \dots, m$, and $c_r = q_{2r}(1)/2^{2r}$ for $r = 1, \dots, k$.

Proof We express the integral as a sum over the m subintervals $[x_{i-1}, x_i]$, $i = 1, \dots, m$, as in (7.13). In the interval $[x_{i-1}, x_i]$ we change the variable by writing $x = x_{i-1} + h(t+1)/2$, so that

$$\int_{x_{i-1}}^{x_i} f(x)\mathrm{d}x = \frac{h}{2}\int_{-1}^{1} g(t)\mathrm{d}t\,,$$

where $f(x) = g(t)$. According to Theorem 7.3, then,

$$\begin{aligned}
&\int_{x_{i-1}}^{x_i} f(x)\mathrm{d}x - \frac{h}{2}[f(x_{i-1}) + f(x_i)] \\
&\quad = \frac{h}{2}\left\{\int_{-1}^{1} g(t)\mathrm{d}t - [g(-1) + g(1)]\right\} \\
&\quad = \frac{h}{2}\left\{\sum_{r=1}^{k} q_{2r}(1)[g^{(2r-1)}(1) - g^{(2r-1)}(-1)]\right. \\
&\qquad\qquad \left. - \int_{-1}^{1} q_{2k}(t)g^{(2k)}(t)\mathrm{d}t\right\}.
\end{aligned}$$

On noting that $g^{(\ell)}(t) = (h/2)^{\ell} f^{(\ell)}(x)$, $\ell = 1, 2, \dots, 2k$, $\mathrm{d}t = (2/h)\,\mathrm{d}x$, summation over all the subintervals $[x_{i-1}, x_i]$, for $i = 1, \dots, m$, gives the required result. The important point is the symmetry of the polynomials q_r, which ensures that $q_{2r}(1) = q_{2r}(-1)$, so that all the derivatives of f at the internal points x_i cancel in the course of summation, leaving only the derivatives at a and b. □

Remark 7.1 *By successively computing the polynomials $q_r(t)$, we can determine the values of $c_r = q_{2r}(1)/2^{2r}$, $r = 1, 2, 3, \dots$. For example,*

$$c_1 = -\tfrac{1}{12}\,,\; c_2 = \tfrac{1}{720}\,,\; c_3 = -\tfrac{1}{30240}\,,\; c_4 = \tfrac{1}{1209600}\,,\; c_5 = -\tfrac{1}{47900160}\,,\dots.$$

It can be shown that $c_r = -\frac{B_{2r}}{(2r)!}$ for all $r = 1, 2, 3, \dots$, where B_{2r} are the Bernoulli numbers[1] with even index, which can be determined from

[1] Jacob Bernoulli the elder (27 December 1654, Basel, Switzerland – 16 August 1705, Basel, Switzerland) was one of the first mathematicians to recognise the significance of the work of Newton and Leibniz on differential and integral calculus. Bernoulli contributed to the theory of infinite series, mechanics, calculus of variations, mechanics, and is also known in probability theory for his Law of Large Numbers.

the Taylor series expansion

$$\tfrac{x}{2}\coth\left(\tfrac{x}{2}\right) = \sum_{r=0}^{\infty} \frac{B_{2r}\, x^{2r}}{(2r)!}\,.$$

Easier still, typing `c[6]=-bernoulli(12)/12!;` *at the Maple command line gives* $c_6 = \frac{691}{1307674368000}$*;* $c_7, c_8, \ldots$ *can be found in the same way.*

An interesting consequence of Theorem 7.4 concerns the numerical integration of smooth periodic functions. Suppose that f is a continuous function defined on $(-\infty, \infty)$ such that all derivatives of f, up to and including order $2k$, are defined and continuous on $(-\infty, \infty)$, and f is periodic on $(-\infty, \infty)$ with period $b - a$; *i.e.*, $f(x + b - a) - f(x) = 0$ for all $x \in \mathbb{R}$. Hence, by successive differentiation of this equality and taking $x = a$ we deduce that, in particular,

$$f^{(2r-1)}(b) - f^{(2r-1)}(a) = 0 \qquad \text{for } r = 1, 2, \ldots, k\,.$$

Therefore, according to (7.20), we have that

$$I - T(m) = \mathcal{O}(h^{2k})\,.$$

The fact that for $k \gg 1$ this integration error is much smaller than the $\mathcal{O}(h^2)$ error that will be observed in the case of a nonperiodic function indicates that the composite trapezium rule is particularly well suited for the numerical integration of smooth periodic functions.

A second application of the Euler–Maclaurin expansion concerns extrapolation methods. This subject will be discussed in the next section.

7.7 Extrapolation methods

In general the calculation of the higher derivatives involved in the Euler–Maclaurin expansion (7.20) is not possible. However, the existence of the expansion allows us to eliminate successive terms by repeated calculation of the trapezium rule approximation.

For example, the case $k = 2$ of (7.20) may be written in the form

$$\int_a^b f(x)\mathrm{d}x - T(m) = C_1 h^2 + \mathcal{O}(m^{-4})\,,$$

where $C_1 = c_1[f'(b) - f'(a)]$ and $h = (b - a)/m$. This also means that

$$\int_a^b f(x)\mathrm{d}x - T(2m) = C_1 (h/2)^2 + \mathcal{O}(m^{-4})\,.$$

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We can eliminate the term in h^2 from these two equalities, giving

$$\int_a^b f(x)\mathrm{d}x = \frac{4T(2m) - T(m)}{3} + \mathcal{O}(h^4)\,.$$

The same elimination process could be used for any two values of m, from the calculation of $T(m_1)$ and $T(m_2)$; the advantage of using m and $2m$ is that in the computation of $T(2m)$ half the required values of $f(x_i)$ are already known from $T(m)$, and we do not have to calculate them again. This process of eliminating the term in h^2 from the expansion of the error is known as **Richardson extrapolation**[1] or h^2 **extrapolation**. It is easy to extend the process to higher-order terms. For example,

$$\int_a^b f(x)\mathrm{d}x - T(m) = C_1h^2 + C_2h^4 + C_3h^6 + \mathcal{O}(h^8)\,.$$

Hence

$$\int_a^b f(x)\mathrm{d}x - \frac{4T(2m) - T(m)}{3} = -\tfrac{1}{4}C_2h^4 - \tfrac{5}{16}C_3h^6 + \mathcal{O}(h^8)\,,$$

which leads to

$$\int_a^b f(x)\mathrm{d}x - \frac{16T_1(2m) - T_1(m)}{15} = \mathcal{O}(h^6)\,,$$

where

$$T_1(m) = \frac{4T(2m) - T(m)}{3}\,.$$

Therefore,

$$T_2(m) = \frac{16T_1(2m) - T_1(m)}{15}$$

approximates the integral $\int_a^b f(x)\mathrm{d}x$ to accuracy $\mathcal{O}(h^6)$. Adopting the notational convention

$$T_0(m) = T(m)$$

and proceeding recursively,

[1] Lewis Fry Richardson (11 October 1881, Newcastle upon Tyne, Northumberland, England – 30 September 1953, Kilmun, Argyllshire, Scotland) studied mathematics, physics, chemistry, botany and zoology at the Durham College of Science, and subsequently Natural Science at King's College in Cambridge. He worked in the National Physical Laboratory and the Meteorological Office, and was the first to apply numerical mathematics, in particular the method of finite differences, to predicting the weather in *Weather Prediction by Numerical Process* (1922). The *Richardson number*, a quantity involving gradients of temperature and wind velocity is named after him.

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Table 7.2. *Romberg table.*

m	$T(m)$	$T_1(m)$	$T_2(m)$	$T_3(m)$	$T_4(m)$
4	$T(4)$	$T_1(4)$	$T_2(4)$	$T_3(4)$	$T_4(4)$
8	$T(8)$	$T_1(8)$	$T_2(8)$	$T_3(8)$	...
16	$T(16)$	$T_1(16)$	$T_2(16)$	...	
32	$T(32)$	$T_1(32)$	...		
64	$T(64)$	...			
...	...				

$$\boxed{T_k(m) = \frac{4^k T_{k-1}(2m) - T_{k-1}(m)}{4^k - 1}, \quad k = 1, 2, 3, \ldots, \qquad (7.21)}$$

will approximate $\int_a^b f(x)\mathrm{d}x$ to accuracy $\mathcal{O}(h^{2k+2})$, provided of course that $f^{(2k+2)}$ exists and is continuous on the closed interval $[a, b]$. This extrapolation process is known as the **Romberg**[1] integration method.

The intermediate results in Romberg's method are often arranged in the form of a table, known as the Romberg table. For example, if we start with $m = 4$ subdivisions of the closed interval $[a, b]$, each of length $h = (b - a)/4$, and proceed by doubling the number of subdivisions in each step (and thereby halving the spacing h between the quadrature points from the previous step), then the associated Romberg table is as shown in Table 7.2, where we took, successively, $m = 4, 8, 16, 32, 64$ subdivisions of the interval $[a, b]$ of length $h = (b - a)/m$ each. After $T_0(4) = T(4), \ldots, T_0(64) = T(64)$ have been computed, we calculate $T_1(4), \ldots, T_1(32)$ using (7.21) with $k = 1$, then we compute $T_2(4), \ldots, T_2(16)$ using (7.21) with $k = 2$, then $T_3(4), T_3(8)$ using (7.21) with $k = 3$, and finally $T_4(4)$ using (7.21) with $k = 4$. Provided that the integrand is sufficiently smooth, the numbers in the $T(m)$ column approximate the integral to within an error $\mathcal{O}(h^2)$; the numbers in the $T_1(m)$ column to within $\mathcal{O}(h^4)$, those in the $T_2(m)$ column to $\mathcal{O}(h^6)$, those in the $T_3(m)$ column to $\mathcal{O}(h^8)$, and those in the $T_4(m)$ column to within $\mathcal{O}(h^{10})$.

[1] Werner Romberg, Emeritus Professor at the Institute of Applied Mathematics at the University of Heidelberg in Germany. The extrapolation process was proposed in his paper Vereinfachte numerische Integration [German], *Norske Vid. Selsk. Forh., Trondheim* **28**, 30–36, 1955.

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An example is shown in Table 7.3. This gives the results of calculating the integral

$$\int_0^1 \frac{\mathrm{e}^{-2x}}{1+4x}\mathrm{d}x$$

by Romberg's method; first the trapezium rule is used successively with $m = 4, 8, 16, 32$ and 64 equal subdivisions of the interval $[0, 1]$ of length $h = (b-a)/m$ each. There are then four stages of extrapolation: Stage 1 involves computing $T_1(m)$ for $m = 4, 8, 16, 32$; Stage 2 computes $T_2(m)$ for $m = 4, 8, 16$; Stage 3 calculates $T_3(m)$ for $m = 4, 8$; and Stage 4 then computes $T_4(m)$ for $m = 4$. Not only does the extrapolation give an accurate result, but the consistency of the numerical values in the last two columns gives a good deal of confidence in quoting the result 0.220458 correct to six decimal digits. Note that none of the individual composite trapezium rule calculations in the $T(m)$ column gives a result correct to more than three decimal digits – not even $T(64)$ which uses 64 equal subdivisions of $[0, 1]$.

Table 7.3. *Romberg table for the calculation of* $\int_0^1 (\mathrm{e}^{-2x}/(1+4x))\mathrm{d}x$.

m	$T(m)$	$T_1(m)$	$T_2(m)$	$T_3(m)$	$T_4(m)$
4	0.248802	0.221038	0.220470	0.220458	0.220458
8	0.227979	0.220505	0.220459	0.220458	
16	0.222374	0.220461	0.220458		
32	0.220940	0.220458			
64	0.220579				

The success of Romberg integration is only justified if the integrand f satisfies the hypotheses of the Euler–Maclaurin Theorem. As an illustration of this, Table 7.4 shows the result of the same calculation, but for the integral

$$\int_0^1 x^{1/3}\mathrm{d}x\,.$$

The function $x \mapsto x^{1/3}$ is not differentiable at $x = 0$, so the required conditions are not satisfied for any extrapolation. The numerical results bear this out; they are quite close to the correct value, 3/4, but the behaviour of the extrapolation does not give any confidence in the accuracy of the result. In fact the extrapolation has not given much improvement

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on $T(64)$. The calculation of integrals involving this sort of singularity requires special methods which we shall not discuss here.

We have reached the end of this chapter, but do not despair: the story about numerical integration rules will continue. In Chapter 10 we shall discuss a class of quadrature formulae, generally referred to as Gaussian quadrature rules, which are distinct from the Newton–Cotes formulae considered here. Before doing so, however, in Chapters 8 and 9 we make a brief excursion into the realm of approximation theory.

Table 7.4. *Romberg table for the calculation of* $\int_0^1 x^{1/3}\mathrm{d}x$.

m	$T(m)$	$T_1(m)$	$T_2(m)$	$T_3(m)$	$T_4(m)$
4	0.708055	0.741448	0.746950	0.748819	0.749534
8	0.733100	0.746606	0.748790	0.749531	
16	0.743230	0.748653	0.749520		
32	0.747297	0.749465			
64	0.748923				

7.8 Notes

The material presented in this chapter is classical. For further details on the theory and practice of numerical integration, we refer to the following texts:

- Philip J. Davis and Philip Rabinowitz, *Methods of Numerical Integration,* Second Edition, Computer Science and Applied Mathematics, Academic Press, Orlando, FL, 1984;
- Vladimir Ivanovich Krylov, *Approximate Calculation of Integrals,* translated from Russian by Arthur H. Stroud, ACM Monograph Series, Macmillan, New York, 1962;
- Hermann Engels, *Numerical Quadrature and Cubature,* Computational Mathematics and Applications, Academic Press, London, 1980.

The first of these is a standard text and contains a huge bibliography of more than 1500 entries. Concerning the implementation of numerical integration rules into mathematical software, the reader is referred to

- Arnold R. Krommer and Christoph W. Ueberhuber, *Computational Integration*, SIAM, Philadelphia, 1998.

It includes a comprehensive overview of computational integration techniques based on both numerical and symbolical methods, and an exposition of some more recent number-theoretical, pseudorandom and lattice algorithms; these topics are beyond the scope of the present text.

Exercises

7.1 With the usual notation for the Newton–Cotes quadrature formula and using the equally spaced quadrature points $x_k = a+kh$ for $k = 0, 1, \ldots, n$ and $n \geq 1$, show that $w_k = w_{n-k}$ for $k = 0, 1, \ldots, n$.

7.2 By considering the polynomial $[x-(a+b)/2]^{n+1}$, $n \geq 1$, and the result of Exercise 1, or otherwise, show that the Newton–Cotes formula using $n+1$ points x_k, $k = 0, 1, \ldots, n$, is exact for all polynomials of degree $n+1$ whenever n is even.

7.3 A quadrature formula on the interval $[-1, 1]$ uses the quadrature points $x_0 = -\alpha$ and $x_1 = \alpha$, where $0 < \alpha \leq 1$:

$$\int_{-1}^{1} f(x)\mathrm{d}x \approx w_0 f(-\alpha) + w_1 f(\alpha)\,.$$

The formula is required to be exact whenever f is a polynomial of degree 1. Show that $w_0 = w_1 = 1$, independent of the value of α. Show also that there is one particular value of α for which the formula is exact also for all polynomials of degree 2. Find this α, and show that, for this value, the formula is also exact for all polynomials of degree 3.

7.4 The Newton–Cotes formula with $n = 3$ on the interval $[-1, 1]$ is

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \approx w_0 f(-1) + w_1 f(-1/3) + w_2 f(1/3) + w_3 f(1)\,.$$

Using the fact that this formula is to be exact for all polynomials of degree 3, or otherwise, show that

$$\begin{aligned} 2w_0 + 2w_1 &= 2\,, \\ 2w_0 + \tfrac{2}{9}w_2 &= \tfrac{2}{3}\,, \end{aligned}$$

and hence find the values of the weights w_0, w_1, w_2 and w_3.

7.5 For each of the functions $1, x, x^2, \ldots, x^6$, find the difference between $\int_{-1}^{1} f(x)\mathrm{d}x$ and (i) Simpson's rule, (ii) the formula derived in Exercise 4.

Deduce that for every polynomial of degree 5 formula (ii) is more accurate than formula (i). Find a polynomial of degree 6 for which formula (i) is more accurate than formula (ii).

7.6 Write down the errors in the approximation of

$$\int_0^1 x^4 \, \mathrm{d}x \quad \text{and} \quad \int_0^1 x^5 \, \mathrm{d}x$$

by the trapezium rule and Simpson's rule. Hence find the value of the constant C for which the trapezium rule gives the correct result for the calculation of

$$\int_0^1 (x^5 - Cx^4) \, \mathrm{d}x \,,$$

and show that the trapezium rule gives a more accurate result than Simpson's rule when $\frac{15}{14} < C < \frac{85}{74}$.

7.7 Determine the values of $c_j, j = -1, 0, 1, 2$, such that the quadrature rule

$$Q(f) = c_{-1} f(-1) + c_0 f(0) + c_1 f(1) + c_2 f(2)$$

gives the correct value for the integral

$$\int_0^1 f(x) \, \mathrm{d}x$$

when f is any polynomial of degree 3. Show that, with these values of the weights c_j, and under appropriate conditions on the function f,

$$\left| \int_0^1 f(x) \, \mathrm{d}x - Q(f) \right| \leq \tfrac{11}{720} M_4 \,.$$

Give suitable conditions for the validity of this bound, and a definition of the quantity M_4.

7.8 Writing $T(m)$ for the composite trapezium rule defined in (7.15) and $S(2m)$ for the composite Simpson's rule defined in (7.17), show that

$$S(2m) = \tfrac{4}{3} T(2m) - \tfrac{1}{3} T(m) \,.$$

7.9 Suppose that the function f has a continuous fourth derivative on the interval $[a, b]$, and that $T(m)$ denotes the composite trapezium rule approximation to $\int_a^b f(x) \mathrm{d}x$, using m subintervals. Show that

$$\frac{T(m) - T(2m)}{T(2m) - T(4m)} \to 4 \quad \text{as } m \to \infty \,.$$

Using the information in Table 7.3 evaluate this expression for $m = 4, 8, 16$.

7.10 With the same notation as in Exercise 9, suppose that the fourth derivative of f is not continuous on $[a,b]$, but that

$$\int_a^b f(x)\mathrm{d}x - T(m) = A/m^\alpha + E(m)\,,$$

where $\alpha > 0$ and A are constants and $\lim_{m\to\infty} m^\alpha E(m) = 0$. Determine

$$\lim_{m\to\infty} \frac{T(m) - T(2m)}{T(2m) - T(4m)}\,.$$

Suggest a value of α which is consistent with the values of $T(m)$ given in Table 7.4.

7.11 The function f has a continuous fourth derivative on the interval $[-1,1]$. Construct the Hermite interpolation polynomial of degree 3 for f using the interpolation points $x_0 = -1$ and $x_1 = 1$. Deduce that

$$\int_{-1}^1 f(x)\mathrm{d}x - [f(-1) + f(1)] = \tfrac{1}{3}[f'(-1) - f'(1)] + E\,,$$

where

$$|E| \le \tfrac{2}{45} \max_{x\in[-1,1]} |f^{iv}(x)|\,.$$

7.12 Construct the polynomials q_4, q_5, q_6 and q_7 given by Definition 7.3. Hence show that, in the notation of Theorem 7.4,

$$c_1 = -1/12\,, \quad c_2 = 1/720\,, \quad c_3 = -1/30240\,.$$

7.13 Using the relations

$$\begin{aligned} 2\sin\tfrac{1}{2}x \sum_{j=1}^m \sin jx &= \cos\tfrac{1}{2}x - \cos(m+\tfrac{1}{2})x\,, \\ 2\sin\tfrac{1}{2}x \sum_{j=1}^m \cos jx &= \sin(m+\tfrac{1}{2})x - \sin\tfrac{1}{2}x\,, \end{aligned}$$

where m is a positive integer, show that the composite trapezium rule (7.15) with m subintervals will give the exact result for each of the integrals

$$\int_{-\pi}^{\pi} \cos rx\,\mathrm{d}x\,, \qquad \int_{-\pi}^{\pi} \sin rx\,\mathrm{d}x\,,$$

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for any integer value of r which is not a multiple of m.

What values are given by the composite trapezium rule for these integrals when $r = mk$ and k is a positive integer?