Last updated: 21 July 2015

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Chapter 7

NUMERICAL INTEGRATION

7.1 Introduction

Definite integrals may be determined *analytically* by the following methods:

(a) Direct integration.

(b) By means of substitution.

(c) Integration by parts.

(d) Using a recursion formula.

(e) Integration in the complex plane.

(f) Series expansion of the integrand.

If none of these methods can be used, then a *numerical method* may be implemented. In this chapter, we consider two techniques based on polynomial interpolation. We also consider the approximation error associated with these techniques, to the extent that we are able to control the accuracy of the approximation.

7.2 Newton-Cotes formulae

The Newton-Cotes formulae for numerical integration, also called interpolatory quadrature, are derived by using *interpolatory polynomial approximations of the integrand.*

Suppose a function $y = f(x)$ is known everywhere on $[x_0, x_n]$. The interval $[x_0, x_n]$ is now divided into n equally sized subintervals, each of length h where

$$h = \frac{x_n - x_0}{n}.$$

The function $y = f(x)$ is approximated by the interpolating polynomial $p_n(x)$ that passes through the points (x_k, y_k), where

$$\begin{aligned} x_k &= x_0 + kh \\ y_k &= f(x_k) \end{aligned}$$

and $k = 0, 1, \ldots, n$. The integral of $p_n(x)$ over $[x_0, x_n]$ is taken as an approximation of $\int_{x_0}^{x_n} f(x)\,\mathrm{d}x$.

Recall from (5.6) we have

$$p_n(x) = \sum_{k=0}^{n} y_k L_k(x)$$

where

$$L_k(x) = \frac{(x - x_0)(x - x_1)\cdots(x - x_{k-1})(x - x_{k+1})\cdots(x - x_n)}{(x_k - x_0)(x_k - x_1)\cdots(x_k - x_{k-1})(x_k - x_{k+1})\cdots(x_k - x_n)}.$$

Since $x_k = x_0 + kh$, it is natural to make the substitution $x = x_0 + sh$, where s is a continuous variable:

$$L_k(s) = \frac{sh(sh-h)\cdots\big[sh-(k-1)h\big]\big[sh-(k+1)h\big]\cdots(sh-nh)}{kh(kh-h)\cdots\big[kh-(k-1)h\big]\big[kh-(k+1)h\big]\cdots(kh-nh)}$$

Both the numerator and denominator are divided by h^n

$$L_k(s) = \frac{s(s-1)\cdots(s-k+1)(s-k-1)\cdots(s-n)}{k(k-1)\cdots(1)(-1)\cdots(k-n)}$$

From the substitution we also have $\mathrm{d}x = h\,\mathrm{d}s$, and so

$$\int_{x_0}^{x_n} p_n(x)\,\mathrm{d}x = \int_0^n \left(\sum_{k=0}^{n} y_k L_k(s)\right) h\,\mathrm{d}s.$$

Since integration is a linear operation the order of integration and summation may be swapped, so that

$$\int_{x_0}^{x_n} p_n(x)\,\mathrm{d}x = (nh)\frac{1}{n}\sum_{k=0}^{n} y_k \int_0^n L_k(s)\,\mathrm{d}s$$

and hence

$$\int_{x_0}^{x_n} f(x)\,\mathrm{d}x \approx \int_{x_0}^{x_n} p_n(x)\,\mathrm{d}x = (x_n - x_0)\sum_{k=0}^{n} C_k^n y_k \tag{7.1}$$

where

$$C_k^n = \frac{1}{n}\int_0^n L_k(s)\,\mathrm{d}s$$

are the so-called *quadrature weights*, sometimes known as the *Cotes numbers*. We will study the *trapezium rule* ($n = 1$) and *Simpson's rule* ($n = 2$).

7.3 Trapezium rule

For $n = 1$ (*linear interpolation*) there are two Cotes numbers

$$C_0^1 = \int_0^1 L_0\,\mathrm{d}s = \int_0^1 \frac{s-1}{0-1}\,\mathrm{d}s = \frac{1}{2}$$
$$C_1^1 = \int_0^1 L_1\,\mathrm{d}s = \int_0^1 \frac{s-0}{1-0}\,\mathrm{d}s = \frac{1}{2}$$

From (7.1) we have

$$\begin{aligned}\int_{x_0}^{x_1} f(x)\,\mathrm{d}x &\approx \frac{1}{2}(x_1 - x_0)(y_0 + y_1)\\ &= \frac{1}{2}(x_1 - x_0)\big[f(x_0) + f(x_1)\big].\end{aligned} \tag{7.2}$$

This is simply the area of the trapezium formed by the interpolation polynomial, the x-axis and the x-intercepts on $[x_0, x_1]$.

If $f(x)$ is nonlinear we might expect the approximation error to be large, particularly if the interval of integration is large. Therefore, to evaluate the integral $\int_a^b f(x)\,\mathrm{d}x$ in a manner which allows the error to be controlled, we subdivide the interval $[a, b]$ into N subintervals, each of length

$$h = \frac{b-a}{N} = \frac{x_N - x_0}{N} \tag{7.3}$$

and the linear approximation (7.2) is performed on *each* of these subintervals. With

$$x_k = x_0 + kh$$
$$y_k = f(x_k)$$

for $k = 0, 1, \ldots, N$, we have

$$\begin{aligned}\int_a^b f(x)\,\mathrm{d}x &\approx \frac{1}{2}h(y_0 + y_1) + \frac{1}{2}h(y_1 + y_2) + \cdots + \frac{1}{2}h(y_{N-1} + y_N) \\ &= \frac{h}{2}(y_0 + 2y_1 + 2y_2 + \cdots + 2y_{N-1} + y_N) \qquad (7.4)\end{aligned}$$

This is known as the *composite trapezium rule*. Equation (7.4) may also be written as

$$\int_a^b f(x)\,\mathrm{d}x \approx \frac{h}{2}\left(y_0 + y_N + 2\sum_{j=1}^{N-1} y_j\right).$$

Approximation error: In order to study the approximation error in the composite trapezium rule, we first obtain an estimate for the error on the first subinterval in (7.4)

$$\Delta_1 = \int_a^{a+h} f(x)\,\mathrm{d}x - \frac{h}{2}\big[f(a) + f(a+h)\big]$$

A Taylor series expansion of $f(x)$ is made about $x = a$:

$$\begin{aligned}\Delta_1 &= \int_a^{a+h}\left[f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!}f''(a) + \cdots\right]\mathrm{d}x \\ &\quad - \frac{h}{2}\big[f(a) + f(a+h)\big] \\ &= [x]_a^{a+h} f(a) + \left[\frac{(x-a)^2}{2}\right]_a^{a+h} f'(a) + \left[\frac{(x-a)^3}{6}\right]_a^{a+h} f''(a) + \cdots \\ &\quad - \frac{h}{2}\big[f(a) + f(a+h)\big] \\ &= hf(a) + \frac{h^2}{2}f'(a) + \frac{h^3}{6}f''(a) + \cdots \\ &\quad - \frac{h}{2}\left[2f(a) + hf'(a) + \frac{h^2}{2}f''(a) + \cdots\right]\end{aligned}$$

To lowest order in h we have

$$\Delta_1 \approx -\frac{h^3}{12}f''(a).$$

For the total approximation error we have

$$\begin{aligned}|\Delta| &\le |\Delta_1| + |\Delta_2| + \cdots + |\Delta_N| \\ &\approx \frac{h^3}{12}\big(|f''(a)| + |f''(a+h)| + \cdots + |f''(a+(N-1)h)|\big) \\ &\le \frac{h^3}{12}NM\end{aligned}$$

where

$$M = \max_{x\in[a,b]} |f''(x)|\,.$$

Thus, we obtain an upper bound for the approximation error

$$|\Delta| \le \frac{h^3}{12}\left(\frac{b-a}{h}\right)M = \frac{h^2\,(b-a)\,M}{12}. \qquad (7.5)$$

Since the computing time is determined by N, it follows from (7.3) that it is wise to make h as large as possible, for a given accuracy. The important term in (7.5) is the power of h. We see that the trapezium rule is a practical computational method, since $\Delta = O(h^2)$.

Example 7.1. Determine

$$I = \int_0^2 e^x \, \mathrm{d}x$$

correct to 4 decimal places.

From (7.5) we have that

$$|\Delta| = \frac{h^2}{12}(2-0)M \leq 10^{-4}$$

where

$$M = \max_{x\in[0,2]} \left| \frac{\mathrm{d}^2}{\mathrm{d}x^2} e^x \right| = e^2.$$

Thus, we obtain an upper bound for the size of each subinterval

$$h \leq \left(\frac{6 \times 10^{-4}}{e^2} \right)^{\frac{1}{2}} = 0.0090$$

and hence a lower bound for the number of subintervals

$$N \geq \frac{2}{h} = 222.22,$$

and so we choose $N = 223$, $h = \frac{2}{223}$. From (7.4) we have

$$\begin{aligned} I_{\text{trap}} &= \frac{1}{2}\left(\frac{2}{223}\right)\left(e^0 + 2e^{\frac{2}{223}} + 2e^{\frac{4}{223}} + \cdots + 2e^{\frac{444}{223}} + e^2\right) \\ &= 6.38910 \end{aligned}$$

Analytically, we find

$$I = e^2 - 1 = 6.38906$$

and we see that the approximation error is of the correct magnitude

$$|\Delta| = |I - I_{\text{trap}}| = 4 \times 10^{-5}.$$

7.4 Simpson's rule

For $n = 2$ (*quadratic interpolation*) there are three Cotes numbers:

$$\begin{aligned} C_0^2 &= \frac{1}{2}\int_0^2 \frac{(s-1)(s-2)}{(0-1)(0-2)} \, \mathrm{d}s = \frac{1}{6} \\ C_1^2 &= \frac{1}{2}\int_0^2 \frac{(s-0)(s-2)}{(1-0)(1-2)} \, \mathrm{d}s = \frac{4}{6} \\ C_2^2 &= \frac{1}{2}\int_0^2 \frac{(s-0)(s-1)}{(2-0)(2-1)} \, \mathrm{d}s = \frac{1}{6} \end{aligned}$$

Equation (7.1) gives the following approximation for the integral:

$$\int_{x_0}^{x_2} f(x) \, \mathrm{d}x \approx (x_2 - x_0)\left(\frac{1}{6}y_0 + \frac{4}{6}y_1 + \frac{1}{6}y_2 \right) \tag{7.6}$$

Again, to determine $\int_a^b f(x) \, \mathrm{d}x$ with error control, it is necessary to subdivide $[a, b]$ into subintervals, and in this case, an even number $2N$. The size of each subinterval is

$$h = \frac{b-a}{2N}.$$

The quadratic approximation is performed on each pair of subintervals. With

$$x_k = x_0 + kh$$
$$y_k = f(x_k)$$

and $k = 0, 1, \ldots, 2N$, it follows from (7.6) that

$$\int_a^b f(x)\,\mathrm{d}x \approx \frac{2h}{6}\big[(y_0 + 4y_1 + y_2) + (y_2 + 4y_3 + y_4) + \cdots + (y_{2N-2} + 4y_{2N-1} + y_{2N})\big]. \tag{7.7}$$

This is known as the *composite Simpson's rule*. Equation (7.7) may also be written as

$$\int_a^b f(x)\,\mathrm{d}x \approx \frac{h}{3}\left(y_0 + y_{2N} + 4y_1 + \sum_{k=1}^{N-1}(2y_{2k} + 4y_{2k+1})\right).$$

Approximation error: Similar to the procedure followed for the composite trapezium rule, we first find the approximation error on the first two subintervals:

$$\Delta_1 = \int_a^{a+2h} f(x)\,\mathrm{d}x - \frac{h}{3}\big[f(a) + 4f(a+h) + f(a+2h)\big]$$

We perform a Taylor expansion of the integrand, $f(a+h)$ and $f(a+2h)$:

$$\begin{aligned}
\Delta_1 = \int_a^{a+2h} &\Bigg[f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!}f''(a) + \frac{(x-a)^3}{3!}f'''(a) \\
&+ \frac{(x-a)^4}{4!}f^{(4)}(a) + \cdots\Bigg]\,\mathrm{d}x - \frac{h}{3}\Bigg[f(a) + 4\bigg(f(a) + hf'(a) + \frac{h^2}{2!}f''(a) \\
&+ \frac{h^3}{3!}f'''(a) + \frac{h^4}{4!}f^{(4)}(a) + \cdots\bigg) + \bigg(f(a) + 2hf'(a) + \frac{(2h)^2}{2!}f''(a) \\
&+ \frac{(2h)^3}{3!}f'''(a) + \frac{(2h)^4}{4!}f^{(4)}(a) + \cdots\bigg)\Bigg] \\
= &\left(2hf(a) + 2h^2f'(a) + \frac{4h^3}{3}f''(a) + \frac{2h^4}{3}f'''(a) + \frac{4h^5}{15}f^{(4)}(a) + \cdots\right) \\
&- \frac{h}{3}\left(6f(a) + 6hf'(a) + 4h^2f''(a) + 2h^3f'''(a) + \frac{5h^4}{6}f^{(4)}(a) + \cdots\right)
\end{aligned}$$

The terms of order h to h^4 cancel identically, and we have to lowest order in h

$$\Delta_1 = -\frac{h^5}{90}f^{(4)}(a).$$

Thus, for the total approximation error on $[a, b]$, we have

$$\begin{aligned}
|\Delta| &\le |\Delta_1| + |\Delta_2| + \cdots + |\Delta_{2N}| \\
&= \frac{h^5}{90}\left(\left|f^{(4)}(a)\right| + \left|f^{(4)}(a+2h)\right| + \cdots + \left|f^{(4)}(a+(2N-2)h)\right|\right) \\
&\le \frac{h^5}{90}NK
\end{aligned}$$

where

$$K = \max_{x\in[a,b]}\left|f^{(4)}(x)\right|. \tag{7.8}$$

Since $hN = \frac{b-a}{2}$, it follows that

$$|\Delta| \le \frac{h^4(b-a)K}{180}. \tag{7.9}$$

We see that

$$\Delta = O(h^4)$$

and Simpson's method is clearly "faster" than the trapezium method, i.e. it will require fewer subintervals to achieve the same accuracy.

Example 7.2. Determine

$$I = \int_0^2 e^x \, \mathrm{d}x$$

correct to 4 decimal places.

From (7.8) we have

$$K = \max_{x \in [0,2]} e^x = e^2$$

and from (7.9) we have

$$h \leq \left(\frac{180\,|\Delta|}{K(b-a)} \right)^{\frac{1}{4}} = \left(\frac{180 \times 10^{-4}}{2e^2} \right)^{\frac{1}{4}} = 0.187$$

and so

$$2N \geq \frac{b-a}{h} = 10.7$$
$$\therefore \quad N \geq 5.35$$

We choose $N = 6$, $h = \frac{2}{12} = \frac{1}{6}$. Equation (7.7) then gives

$$\int_0^2 e^x \, \mathrm{d}x \approx \frac{1}{18} \left[e^0 + e^2 + 4 \left(e^{\frac{1}{6}} + e^{\frac{3}{6}} + \cdots + e^{\frac{11}{6}} \right) + 2 \left(e^{\frac{2}{6}} + e^{\frac{4}{6}} + \cdots + e^{\frac{10}{6}} \right) \right]$$
$$= 6.38908$$

We compare the Simpson approximation with the exact value of the integral

$$|\Delta| = |I - I_{\text{Simpson}}| = 2.7 \times 10^{-5}$$

We see that the error is as expected $\left(\leq 10^{-4}\right)$. We also see that Simpson's method only requires 13 evaluations of $f(x)$, whereas the Trapezium rule required 223 such evaluations.

7.5 An analytical complication

If $\int_a^b f(x)\,\mathrm{d}x$ exists but the integrand $f(x)$ does not exist somewhere on $[a, b]$, then the numerical evaluation of the integral requires particular care. We consider this case by way of an example.

Example 7.3. Determine

$$I = \int_0^1 x^{-\frac{1}{2}} \cos x \, \mathrm{d}x.$$

The integrand $f(x) = \frac{\cos x}{\sqrt{x}}$ does not exist at $x = 0$, and so the integral cannot be determined using either the Trapezium rule or Simpson's rule. However, the singularity at $x = 0$ is of the form $x^{-\frac{1}{2}}$ and the integral does indeed exist. To facilitate numerical evaluation we first integrate by parts:

$$I = \left[2x^{\frac{1}{2}} \cos x \right]_0^1 + \int_0^1 2x^{\frac{1}{2}} \sin x \, \mathrm{d}x = 2\cos 1 + \ I_1$$

where the integrand in

$$I_1 = \int_0^1 2x^{\frac{1}{2}} \sin x \, \mathrm{d}x$$

exists everywhere on $[0, 1]$ and so I_1 may be determined numerically.