Chapter 5

Numerical Integration in One Variable

Introduction

Numerical integration of a function of a single variable is a highly developed technique. As in using a vending machine, we can choose what we need by pressing the appropriate button; so too in numerical integration, one has a choice of several very efficient computer programs. One can indeed reduce the choice to the Gauss integration schemes that work very well for a wide range of smooth functions, and even integrate functions that have mild discontinuities within the interval of integration—at a somewhat greater cost.

Digital computers free us from the labor of tedious calculations; but judgement is still called for in the use of numerical integration procedures if we wish to compute economically. The following situations are typical:

(i) we may need only a rough approximation to the value of the integral;

(ii) the integral can be expressed in closed form, but this form is not convenient for computation; and

(iii) the problem that gave rise to the integral may be more conveniently solved by other means.

Illustrations of these situations are given below. In particular, it is desirable to emphasize the value of rough approximations that can be obtained quickly. These are particularly valuable to the beginning student who is intent on finding out why certain procedures work well, and when. Furthermore, rough approximations are often desirable before undertaking extensive and expensive calculations.

In this chapter, considerable space is given to elementary methods that are useful for quick approximations, and also to methods based on the Euler-Maclaurin formula—although this formula is rarely used to evaluate integrals, it helps us to understand the success or failure of different methods. In contrast, much of the detailed analysis of Gaussian methods is omitted, since it is already available in many texts, and since it offers very little towards the understanding of practical difficulties.

5.1 Typical Examples

This section consists of a number of simple examples that illustrate the need for the user to think, and to proceed with caution.

Example 5.1.1 If $n > 2$, the integral

$$I(n) = \int_0^1 \frac{dx}{(1+x^n)^{1/2}}$$

cannot be expressed as an elementary function of n. However, $I(n)$ can be approximated numerically by many different methods.

The integral

$$J(n) = \int_0^1 \frac{dx}{(1-x^n)^{1/2}} \;, \quad n = 3, 4, 5, \ldots$$

is more difficult since it has an integrable singularity at $x = 1$. Integration by parts makes the numerical approximation of $J(n)$ more tractible. Setting

$$F(x) = \frac{1-x^n}{1-x}$$

and noting that $F(0) = 1$, we get

$$\begin{aligned} J(n) &= \int_0^1 (1-x)^{-1/2} F(x)^{-1/2} dx \\ &= 2 - \int_0^1 (1-x)^{1/2} F(x)^{-3/2} F'(x) dx \,. \end{aligned}$$

Example 5.1.2 It is sometimes possible to express the integral in closed form, in which case numerical integration is pointless. For example, it can be shown that

$$I = \int_0^\infty e^{-ax^2} \cos bx \, dx = \frac{1}{2}\left(\frac{\pi}{a}\right)^{1/2} \exp\left(-\frac{b^2}{4a}\right) \;, \quad a > 0 \,.$$

This closed form expression can be very useful, since it illustrates the dependence of I on a and b, and can therefore lead to a useful numerical method of approximating

$$\int_0^y e^{-ax^2} \cos bx\, dx$$

when y is finite.

Example 5.1.3 The integral

$$S(x) = \int_0^\infty e^{-t^2} \sin xt\, dt \tag{5.1.1}$$

cannot be expressed as a finite combination of elementary functions. If we differentiate the integral with respect to x, and integrate by parts, we obtain the differential equation

$$\frac{dS}{dx} = \frac{1}{2} - \frac{1}{2} x\, S(x)\ , \quad S(0) = 0\,, \tag{5.1.2}$$

whose solution is given as a power series in x:

$$S(x) = \sum_{k=0}^{\infty} \frac{(-1)^k k\,!}{2(2k+1)\,!}\, x^{2k+1}\ , \quad |x| < \infty\,. \tag{5.1.3}$$

Five terms of the series (5.1.3) yield an accuracy of two significant figures if $|x| \leq 2$. We can also show that

$$S(x) = \frac{1}{x} + O\left(\frac{1}{x^3}\right) \tag{5.1.4}$$

as $x \to \infty$, and this information may be sufficient to solve the problem. If more accuracy is required we can use a Gaussian integration method.

Example 5.1.4

$$I = \int_0^x \frac{tdt}{a^3 + t^3} = \frac{1}{6a} \ln\left[\frac{x^2 - ax + a^2}{(x+a)^2}\right] + \frac{1}{a\sqrt{3}} \operatorname{arc}\left(\tan\left(\frac{x\sqrt{3}}{2a - x}\right)\right)\,. \tag{5.1.5}$$

If the integral is to be evaluated for a single value of x and a, then the expression on the right is the most suitable method of computation. If I is required for several values of x and a, then numerical integration is preferable. Setting $t = xs$, $a = xb$ in (5.1.5), we get

$$I = \frac{1}{x}\int_0^1 \frac{sds}{b^3 + s^3} = \frac{2}{x}\int_{-1}^1 \frac{(1+v)dv}{8b^3 + (1+v)^3}\,, \tag{5.1.6}$$

where s has further been replaced by $(1+v)/2$ on the right.

Example 5: The differential equation

$$\frac{dy}{dx} = \frac{2y}{1 - x^4} \tag{5.1.7}$$

may be explicitly solved by method of separation of variables, by writing it in the form

$$\int \frac{dy}{y} = 2\int \frac{dx}{1-x^4}\,.$$

Upon decomposing $(1-x^4)^{-1}$ into partial fractions, we find that (5.1.7) has the solution

$$y = A\left(\frac{1+x}{1-x}\right)^{1/2} e^{u(x)} \tag{5.1.8}$$

where A is a constant, and $u(x) = \arctan x$. This expression for y, although somewhat cumbersome, can be readily evaluated. However, if we add x to the right of (5.1.7), we get

$$\frac{dy}{dx} = \frac{2y}{1-x^4} + x\,; \tag{5.1.9}$$

the solution of (5.1.9) using standard differential equation methods is

$$y = \left(\frac{1+x}{1-x}\right)^{1/2} e^{u(x)}\left[A + \int_0^x t\left(\frac{1-t}{1+t}\right)^{1/2} e^{-u(t)}dt\right]. \tag{5.1.10}$$

The integral on the right cannot be expressed in closed form, and it is moreover inconvenient for numerical evaluation. It is preferable, for solving (5.1.9), to use a numerical method of solving differential equations on (5.1.9) directly rather than to use a numerical method of approximating the integral in (5.1.10). When faced with a very cumbersome integral, it is often advisable to ask where it came from.

Example 5.1.5 The integral

$$J_n(x) = \frac{1}{\pi}\int_0^\pi \cos(x\cos\theta - n\theta)d\theta \tag{5.1.11}$$

can be easily evaluated numerically for moderate values of x and n, although numerical integration may be less efficient than the evaluation of $J_n(x)$ by use of the series

$$J_n(x) = \left(\frac{x}{2}\right)^n \sum_{k=0}^{\infty} \frac{(-x^2/4)^k}{k\,!\,(n+k)\,!}\,, \quad |x| < \infty\,. \tag{5.1.12}$$

If x or n (or both) are large, then the integrand in (5.1.11) oscillates very rapidly, and it is then preferable to use the asymptotic methods of Chapter 6.

Example 5.1.6 The integrals

$$\int_0^\infty \cos(ax^2)dx = \frac{1}{2}\left(\frac{\pi}{2a}\right)^{1/2}, \quad \int_0^\infty \sin(ax^2)dx = \frac{1}{2}\left(\frac{\pi}{2a}\right)^{1/2}, \tag{5.1.13}$$

converge because the integrand in each oscillates increasingly rapidly as x increases and the positive and negative contributions tend to cancel more and more for large x. The conditional convergence of each integral can be readily illustrated by means of the transformation $t = ax^2$. A numerical integration procedure that does not take account of the oscillation phenomenon of the integrands may yield poor results when applied to the numerical approximation of integrals of a similar type to (5.1.13).

Problems

5.1.1 Use the power series expansion of $S(x)$ in (5.1.1) and integrate termwise to get (5.1.3).

5.1.2 Either use integration by parts along with (5.1.1) or substituion along with (5.1.2) to show that

$$S(x) \sim \sum_{n=0}^{\infty} \frac{(-1)^n n!}{x^{2n+1}}$$

5.1.3 How many terms of the series (5.1.3) are required to evaluate to an accuracy of three significant figures for $|x| \leq 10$?

5.1.4 Prove that the function

$$A(x) = \int_0^\infty e^{-t^3 - xt}\, dt$$

can be computed for intermediate and small values of x by means of the power series

$$A(x) = \frac{1}{3}\sum_{n=0}^{\infty} \frac{\Gamma\left(\frac{n+1}{3}\right)}{n!}(-1)^n x^n$$

while for large values of x, the asymptotic expansion

$$A(x) \sim \sum_{n=0}^{\infty} \frac{(-1)^n (3n)!}{n!\, x^{3n+1}}$$

is useful.

5.1.5 Prove that the function $f(x)$ defined by the integral

$$f(x) = \int_0^\infty \frac{e^{-u^2}}{x+u}\,du \quad , \quad x > 0$$

satisfies the differential equation $f' - 2xf = \pi^{1/2} - \dfrac{1}{x}$. Use this equation to deduce that

$$f(x) \sim \frac{1}{2}\sum_{n=0}^{\infty} \frac{(-1)^n \Gamma\left(\frac{n+1}{2}\right)}{x^{n+1}}$$

and also, that the function $y = f(x) + e^{-x^2}\log x$ satisfies the differential equation

$$y' + 2xy = \pi^{1/2} - \frac{1-e^{-x^2}}{x} = \pi^{1/2} + \sum_{n=1}^{\infty} \frac{(-1)^n x^{2n-1}}{n\,!}\,,$$

whose solution is $y = \sum_{n=0}^{\infty} a_n x^n$ with $a_0 = -\frac{1}{2}\tau$, where τ is Euler's constant, i.e.

$$\tau = \lim_{k\to\infty}\left[\sum_{n=1}^{k} \frac{1}{n} - \ln(k)\right] = .577215665\,.$$

5.1.6 Use the identity

$$I = \int_0^\infty J_0(t)e^{-pt}dt = (1+p^2)^{-1/2}$$

which is obtainable from a table of Laplace transforms, to deduce that

$$\int_0^\infty J_0(t)dt = 1\,.$$

(Here J_0 is the Bessel function of order zero.) Can the transform

$$\int_0^\infty e^{-pt}\sin(t)dt = \frac{1}{1+p^2}$$

be used similarly?

5.2 The Equi-Spaced Midordinate and Trapezoidal Rules

The methods of this section are very simple, and very general. They are mainly used to obtain rough approximations, although they can be modified to yield more accurate approximations.

If $f(x)$ is continuous on the interval $[0,1]$, and if $f''(x)$ exists on the interval $(0,1)$, then it follows from Taylor's theorem that

$$f(x) = f\left(\frac{1}{2}\right) + \left(x - \frac{1}{2}\right) f'\left(\frac{1}{2}\right) + \frac{1}{2}\left(x - \frac{1}{2}\right)^2 f''(\zeta) \quad , \quad 0 \le x \le 1 \, , \tag{5.2.1}$$

where ζ is between $1/2$ and x. Integrating both sides of (5.2.1), we get

$$\begin{aligned} \int_0^1 f(x)dx &= f\left(\frac{1}{2}\right) + \frac{1}{2}\int_0^1 \left(x - \frac{1}{2}\right)^2 f''(\zeta)dx \\ &= f\left(\frac{1}{2}\right) + \frac{1}{2} f''(\xi) \int_0^1 \left(x - \frac{1}{2}\right)^2 dx \\ &= f\left(\frac{1}{2}\right) + \frac{1}{24} f''(\xi) \, . \end{aligned} \tag{5.2.2}$$

In the second step of (5.2.2) we have used the mean value theorem for integrals, so that ξ is between 0 and 1. This yields the simplest form of the midordinate rule.

Example 5.2.1

$$I = \int_0^1 e^{-1/2\, x^2} dx = e^{-1/8} - \frac{1}{24}(1 - \xi^2) e^{-1/2\, \xi^2}$$

for some $\xi \in (0,1)$. Notice that the error of approximating the integral by $e^{-1/8}$ is negative and bounded by $1/24 \cong .0416$. This bound is quite close to the exact error, since

$$I \cong .8557\ldots \; , \quad e^{-1/8} = .8825\ldots \; ,$$

so that the error, $I - e^{-1/8} \cong -.0262$.

The trapezoidal formula is obtained by a slightly different device. By means of Lagrange's interpolation formula we get

$$f(x) = (1-x)f(0) + xf(1) - \frac{x(1-x)}{2} f''(\zeta) \; , \quad 0 \le x \le 1 \, . \tag{5.2.3}$$

Integrating both sides of (5.2.3), and using the mean value theorem, we obtain

$$\int_0^1 f(x)dx = \frac{1}{2}[f(0)+f(1)] - \frac{1}{12}f''(\xi) \tag{5.2.4}$$

for some $\xi \in (0,1)$. This is the simplest form of the trapezoidal rule.

Note that the error of (5.2.2) is $(1/24)f''(\xi_1)$ while the error of (5.2.4) is $-(1/12)f''(\xi_2)$ (in general, $\xi_1 \neq \xi_2$). *If $f''(x)$ has the same sign throughout $(0,1)$, then the errors of (5.2.2) and (5.2.4) are of opposite sign, and the magnitude of the difference bounds the error of each approximation,* i.e.

$$\begin{aligned}
\left|\int_0^1 f(x)dx - \frac{1}{2}[f(0)+f(1)]\right| &\leq \left|f\left(\frac{1}{2}\right) - \frac{1}{2}[f(0)+f(1)]\right| \\
\left|\int_0^1 f(x)dx - f\left(\frac{1}{2}\right)\right| &\leq \left|f\left(\frac{1}{2}\right) - \frac{1}{2}[f(0)+f(1)]\right|.
\end{aligned} \tag{5.2.5}$$

Example 5.2.2 Approximation of the integral of Example 5.2.1 by the trapezoidal rule (5.2.4) yields

$$\int_0^1 e^{-1/2\,x^2}dx = \frac{1}{2}(1+e^{-1/2}) + \frac{1}{12}(1-\xi^2)e^{-1/2\,\xi^2}$$

for some $\xi \in (0,1)$. The error of approximating the integral by the first term on the right is bounded by $1/12 \cong .0833$; the exact error is .0524.

The average of the midordinate and trapezoidal results is $1/2[.8825 + .8023] \cong .8424$, and the error of this average is .0103. It may be shown that this error is less than the two preceding errors, since the second derivative of the integrand has the same sign throughout the interval.

Problems

5.2.1 Show that

(a) $\frac{1}{2} \leq \int_0^1 (1-x^2)^{1/2}dx \leq \left(\frac{3}{4}\right)^{1/2}$

(b) $\frac{1}{2}[\tan^{-1}(1) + \tan^{-1}(2)] \leq \int_0^1 \tan^{-1}(1+x)dx \leq \tan^{-1}\left(\frac{3}{2}\right)$.

5.2.2 Verify the statements in the last paragraph of the chapter for the integral

$$I = \int_0^1 \ln(x+1)dx = 2\ln 2 - 1\,.$$

That is, approximate I via the midordinate and trapezoid rules, respectively.

5.3 Transformation of the Integral: Composite Rules

Let us consider the evaluation of

$$I = \int_a^b f(y)dy \tag{5.3.1}$$

where a and b are finite, $f(y)$ is continuous on $[a,b]$, and $f''(y)$ exists on (a,b). By means of the transformation

$$y = a + (b-a)x \,, \tag{5.3.2}$$

(5.3.1) becomes

$$I = (b-a)\int_0^1 f[a+(b-a)x]dx \,. \tag{5.3.3}$$

Noticing that

$$\frac{d^2}{dx^2} f[a+(b-a)x] = (b-a)^2 \frac{d^2 f(y)}{dy^2}$$

and using the notation

$$f''(y) = \frac{d^2}{dy^2} \,,$$

we can deduce from (5.2.2) and (5.2.4) that

$$\begin{aligned} \int_a^b f(y)dy &= (b-a) f\left(\frac{a+b}{2}\right) + \frac{(b-a)^3}{24} f''(\zeta) \\ &= \frac{(b-a)}{2}[f(a)+f(b)] - \frac{(b-a)^3}{12} f''(\xi) \end{aligned} \tag{5.3.4}$$

where ζ and ξ are points located on (a,b).

We can now obtain a more accurate approximation of $\int_0^1 f(x)dx$, by dividing the interval $[0,1]$ into n subintervals and applying one of (5.3.4) over each subinterval. Let j and n be positive integers such that $j \le n$. Then (5.3.4) yields

$$\begin{aligned} \int_{(j-1)/n}^{j/n} f(x)dx &= \frac{1}{n} f\left(\frac{2j-1}{2n}\right) + \frac{1}{24n^3} f''(\zeta_j) \\ &= \frac{1}{2n}\left[f\left(\frac{j-1}{n}\right) + f\left(\frac{j}{n}\right)\right] - \frac{1}{12n^3} f''(\xi_j) \end{aligned} \tag{5.3.5}$$

where ζ_j and ξ_j are located in $((j-1)/n, j/n)$.

Summing both sides of (5.3.5) over j, from 1 to n, we obtain

$$\begin{aligned}\int_0^1 f(x)dx &= \sum_{j=1}^{n} \int_{(j-1)/n}^{j/n} f(x)dx \\ &= M_n(f) + \frac{\epsilon_n}{24n^2} \quad \text{(midordinate)} \\ &= T_n(f) - \frac{\delta_n}{12n^2} \quad \text{(trapezoidal)}\end{aligned} \tag{5.3.6}$$

where

$$\begin{aligned} M_n(f) &= \frac{1}{n}\left[f\left(\frac{1}{2n}\right) + f\left(\frac{3}{2n}\right) + \cdots + f\left(\frac{2n-1}{2n}\right)\right] \\ T_n(f) &= \frac{1}{n}\left[\frac{1}{2}f(0) + f\left(\frac{1}{n}\right) + \cdots + f\left(\frac{n-1}{n}\right) + \frac{1}{2}f(1)\right]\end{aligned} \tag{5.3.7}$$

and where

$$\begin{aligned} \epsilon_n &= \frac{1}{n}[f''(\zeta_1) + f''(\zeta_2) + \cdots + f''(\zeta_n)] \\ \delta_n &= \frac{1}{n}[f''(\xi_1) + f''(\xi_2) + \cdots + f''(\xi_n)]\,. \end{aligned} \tag{5.3.8}$$

We now observe that ϵ_n is the average of the n values of $f''(\zeta_j)$, $j = 1, 2, \ldots, n$; hence if $f''(x)$ exists on $(0,1)$ there exists a point ζ such that

$$\epsilon_n = f''(\zeta)\ , \quad \zeta \in (0,1)\,.$$

Similarly, there exists a point ξ such that

$$\delta_n = f''(\xi)\ , \quad \xi \in (0,1)\,.$$

We have thus proved

Theorem 5.3.1 *Let $f(x)$ be continuous on the interval $[0,1]$, and let $f''(x)$ exist on $[0,1]$. Then*

$$\begin{aligned}\int_0^1 f(x)dx &= M_n(f) + \frac{1}{24n^2}f''(\zeta) \\ &= T_n(f) - \frac{1}{12n^2}f''(\xi)\end{aligned} \tag{5.3.9}$$

where M_n and T_n are defined in (5.3.7), and ζ and ξ are points on $(0,1)$.

From this theorem, and from the definitions of M_n and T_n, we deduce, as in (5.2.5):

Corollary 5.3.2 *If $f(x)$ is continuous on $[0,1]$ and $f''(x)$ exists and does not change sign on $(0,1)$, then*

$$\begin{aligned} \left| \int_0^1 f(x)dx - M_n(f) \right| &\leq |T_n(f) - M_n(f)| \\ \left| \int_0^1 f(x)dx - T_n(f) \right| &\leq |T_n(f) - M_n(f)| \,. \end{aligned} \tag{5.3.10}$$

We note furthermore, from the definition of T_n and M_n, that

$$T_{2n} = \frac{1}{2}[T_n + M_n]\,. \tag{5.3.11}$$

Theorem 5.3.1 has a simple geometric interpretation. The condition $f''(x) > 0$ on $(0,1)$ implies that $f(x)$ is convex on the interval $[0,1]$. Since a convex function lies below its chord, it is clear that

$$\int_0^1 f(x)dx < \frac{1}{2}[f(0) + f(1)]\ , \text{ and } f\left(\frac{1}{2}\right) < \int_0^1 f(x)dx\,.$$

These inequalities are illustrated in Figure 5.3.1.

Figure 5.3.1: A convex function

If $f(x)$ decreases for $x \geq 0$, then

$$f(1) + f(2) + \cdots + f(n) \leq \int_0^n f(x)dx \leq f(0) + f(1) + \cdots + f(n-1)\,,$$

the inequality being strict if $f(x)$ is strictly decreasing.

Many integration rules exist that are based on the evaluation of $f(x)$ at equi-spaced points. Very well known among these are Simpson's rule and Weddle's rule. Simpson's rule takes the form

$$\int_a^b f(x)dx = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] - \frac{(b-a)^5}{2880} f^{(4)}(\zeta)\,. \quad (5.3.12)$$

Composite Simpson's rules require that the interval be divided into an even number of strips, since the rule (5.3.12) uses three equi-spaced points, or two strips of length $(b-a)/2$. Weddle's is defined by

$$\begin{aligned}\int_a^b f(x)dx \;=\; & \frac{3h}{10}[\{f(a) + f(b)\} + 5\{f(a+h) + f(a+5h)] \\ & +\{f(a+2h) + f(a+4h)\} + 6f(a+3h) \qquad (5.3.13) \\ & -\frac{(b-a)^6}{6,531,840} f^{(6)}(\zeta)\,, \quad a < \zeta < b\,, \quad h = \frac{b-a}{6}\,.\end{aligned}$$

It involves six intervals of equal length, and seven evaluation points.

The formulas (5.3.12) and (5.3.13) were quite popular a few years ago, because of their simplicity, and because of the small coefficient of the error term. Weddle's rule may also be used to check Simpson's rule of every third step. Despite these advantages, the above rules are used little, save in rough approximations.

Corollary 5.3.2 suggests the following algorithm for computing $\int_0^1 f(x)dx$, when $f''(x)$ is of one sign on the interval $(0,1)$.

Algorithm 5.3.3 Quadrature Based on T_n and M_n

ϵ given
Evaluate T_1
$n = 1$
    Evaluate M_n
        If $|T_n - M_n| < \epsilon$, print T_n or M_n
        If $|T_n - M_n| \geq \epsilon$
    $T_{2n} = 1/2(T_n + M_n)$
$n \to 2n$
Return

Problems

5.3.1 Approximate

(a) $\frac{\pi}{4} = \int_0^1 (1-x^2)^{1/2} dx$

(b) $\int_0^1 \log(1+x) dx$

by $T_n((1-x^2)^{1/2})$ and by $M_n((1-x^2)^{1/2})$, for $n = 1, 2, 4, 8, 16$.

5.3.2 For the function $f(x) = (1-x)^{1/2}$, find positive constants c_1 and c_2 such that

$$\frac{c_1}{n^{3/2}} \leq \int_0^1 f(x) dx - T_n(f) \leq \frac{c_2}{n^{3/2}} .$$

5.4 The Euler-Maclaurin Formula

The Euler-Maclaurin formula is used little in applications, and our present treatment of it is therefore brief. Our treatment of this formula helps us explain why the trapezoidal and midordinate rules are sometimes so remarkably accurate, and it helps us explain the Romberg algorithm in Section 5.5, as well as the formulas of Section 5.6.

If we apply Taylor's formula

$$\begin{aligned} F(x) &= F(a) + (x-a)F'(a) + \cdots + \frac{(x-a)^{n-1}}{(n-1)\,!} F^{(n-1)}(a) \\ &\quad + \frac{1}{(n-1)\,!} \int_a^x (x-t)^{n-1} F^{(n)}(t) dt \end{aligned}$$

to the function $F(x) = \int_0^x f(t) dt$ then

$$\int_0^x f(t) dt = x f(0) + \int_0^x (x-t) f(t) dt . \tag{5.4.1}$$

Similarly, applying Taylor's formula to $G(u) = \int_1^u f(t) dt$, we get

$$\int_1^u f(t) dt = (u-1) f(1) + \int_1^u (u-t) f(t) dt . \tag{5.4.2}$$

Now by taking $x = 1$ in (5.4.1), $u = 0$ in (5.4.2), and adding the results, we get

$$\int_0^1 f(t) dt = \frac{1}{2}[f(0) + f(1)] + \int_0^1 \left(\frac{1}{2} - t\right) f'(t) dt . \tag{5.4.3}$$

Let us set

$$P_1(x) = \frac{1}{2} - x \; , \;\; 0 \leq x < 1 \; , \;\; P_1(1+x) = P_1(x) \; , \;\; \forall x \, . \tag{5.4.4}$$

With the notation $[x] =$ largest integer $\leq x$ the function $P_1(x)$ is given by

$$P_1(x) = -x + [x] + \frac{1}{2} \; , \quad \forall x \, . \tag{5.4.5}$$

This is graphed in Figure 5.4.1. It can be shown that $P_1(x)$ has a Fourier

Figure 5.4.1: $P_1(x) = -x + [x] + 1/2$

series expansion, given by

$$P_1(x) = \sum_{n=1}^{\infty} \frac{2\sin(2\pi n x)}{2\pi n} \, . \tag{5.4.6}$$

Integrating this series, and requiring $P_2(0) = P_2(1)$, we obtain

$$P_2(x) = -\sum_{n=1}^{\infty} \frac{2\cos(2\pi n x)}{(2\pi n)^2} \, .$$

Again, integrating this result and requiring $P_3(0) = P_3(1) = 0$ leads to

$$P_3(x) = -\sum_{n=1}^{\infty} \frac{2\sin(2\pi n x)}{(2\pi n)^3} \, .$$

Repeating these steps and requiring $P_{2r}(0) = P_{2r}(1)$ and $P_{2r+1}(0) = P_{2r+1}(1) = 0$ leads to the identities

$$\begin{aligned} P_{2r}(x) &= (-1)^r \sum_{n=1}^{\infty} \frac{2\cos(2\pi n x)}{(2\pi n)^{2r}} \\ P_{2r+1}(x) &= (-1)^r \sum_{n=1}^{\infty} \frac{2\sin(2\pi n x)}{(2\pi n)^{2r+1}}\,, \end{aligned} \tag{5.4.7}$$

$r = 1, 2, 3, \ldots$. We also deduce the following three relationships at once; that is

$$\begin{aligned} P_r(1-x) &= (-1)^r P_r(x) \\ (-1)^r P_{2r}(0) &> |P_{2r}(x)|\ , \quad 0 < x < 1\,, \end{aligned}$$

and

$$\begin{aligned} P_{2r}(x) - P_{2r}(0) &= (-1)^{r-1} \sum_{n=1}^{\infty} \frac{2[1-\cos(2\pi n x)]}{(2\pi n)^{2r}} \\ &= (-1)^{r-1} \sum_{n=1}^{\infty} \frac{4\sin^2(\pi n x)}{(2\pi n)^{2r}} \end{aligned} \tag{5.4.8}$$

Note that $P_{2r}(x) - P_{2r}(0) = 0$ for $x = 0$ and 1, and therefore $P_{2r}(x) - P_{2r}(0)$ assumes its largest modulus at $x = 1/2$. Further:

(i) It may be shown, using (5.4.7), that $P_{2r}(x)$ is an even function of $x - 1/2$ and $P_{2r+1}(x)$ an odd function of $x - 1/2$, and so $P_{2r+1}(1/2) = 0$.

(ii) Using (5.4.7) we can show that

$$P_{2r}\left(\frac{1}{2}\right) - P_{2r}(0) = -(1 - 2^{1-2r}) P_{2r}(0)\,. \tag{5.4.9}$$

(iii) The numbers $P_{2r}(0)$ alternate in sign.

We remark that the functions $P_r(x)$ are related to the Bernoulli polynomials $B_r(x)$ (c.f. the problems at the end of this section) by the equation

$$-P_r(x) = \frac{B_r(x)}{r\,!}\ , \quad 0 \le x \le 1\,. \tag{5.4.10}$$

It is moreover useful to note that

$$-P_{2r}(1) = -P_{2r}(0) = (-1)^{r+1}\sum_{n=1}^{\infty}\frac{2}{(2\pi n)^{2r}} = \frac{B_{2r}(0)}{(2r)\,!} = \frac{B_{2r}}{(2r)\,!} \tag{5.4.11}$$

where B_{2r} is the $2r^{\text{th}}$ Bernoulli number.

Integrating the extreme right of (5.4.3) by parts and using (5.4.5), we obtain:

Theorem 5.4.1 *Let $f^{(2m)}(x)$ be continuous on the interval $[0,1]$. Then*

$$\begin{aligned}\int_0^1 f(x)dx &= \frac{1}{2}[f(0)+f(1)] + \sum_{k=1}^{m}\frac{B_{2k}}{(2k)\,!}[f^{(2k-1)}(0) - f^{(2k+1)}(1)] \\ &\quad + \int_0^1 \frac{B_{2m}(x)}{(2m)\,!}\,f^{(2m)}(x)dx\,.\end{aligned} \tag{5.4.12}$$

We next use Theorem 5.4.1 and the transformation method of Section ????2.3 to obtain the formula

$$\begin{aligned}\int_{j-1/n}^{j/n} f(x)dx &= \frac{1}{2n}\left[f\left(\frac{j-1}{n}\right) + f\left(\frac{j}{n}\right)\right] \\ &\quad + \sum_{k=1}^{m}\frac{B_{2k}}{n^{2k}(2k)\,!}\left[f^{(2k-1)}\left(\frac{j-1}{n}\right) - f^{(2k-1)}\left(\frac{j}{n}\right)\right] \\ &\quad + \int_{j-1/n}^{j/n}\frac{B_{2m}(nx-j+1)}{n^{2m+1}}\,f^{(2m)}(x)dx\,.\end{aligned} \tag{5.4.13}$$

Upon summing (5.4.13) with respect to j from 1 to n, we arrive at:

Theorem 5.4.2 *Let $f^{(2m)}(x)$ be continuous on the interval $[0,1]$. Then*

$$\begin{aligned}\int_0^1 f(x)dx &= T_n(f) + \sum_{k=1}^{m}\frac{B_{2k}}{n^{2k}((2k)\,!}[f^{(2k)}(0) - f^{(2k)}(1)] \\ &\quad + \frac{1}{n^{2m+1}}\int_0^1 P_{2m}(nt)f^{(2m)}(t)dt,.\end{aligned} \tag{5.4.14}$$

where $T_n(f)$ is defined in (5.3.7).

Proof: See Problem 5.4.5.

The coefficients $|B_{2k}/(2k)\,!|$ in the correction term decrease rapidly when k is large; from (5.4.7) we see that

$$\left|\frac{B_{2k}}{(2k)\,!}\right| = |P_{2k}(0)| \cong \frac{2}{(2\pi)^{2k}},. \tag{5.4.15}$$

Moreover $P_{2k+2}(0)/P_{2k}(0) \cong 1/40$. The first five coefficients are given in Table 5.4.1.

Table 5.4.1: The Coefficients $P_{2k}(0)$.

k	1	2	3	4	5
$-P_{2k}(0) = \frac{B_{2k}}{(2k)!}$	$\frac{1}{12}$	$-\frac{1}{720}$	$\frac{1}{30{,}240}$	$-\frac{1}{1{,}209{,}600}$	$\frac{1}{47{,}900{,}160}$

We note in particular, that the right-hand side of (5.4.14) is an asymptotic expansion of $\int_0^1 f(x)dx$ as $n \to \infty$. For the first few terms of this Table 5.4.1 records

$$\begin{aligned}\int_0^1 f(x)dx \;=\; & T_n(f) - \frac{1}{12n^2}\,[f'(1) - f'(0)] \\ & + \frac{1}{240n^4}\,[f^{(3)}(1) - f^{(3)}(0)] - \frac{1}{30,240}[f^{(5)}(1) - f^5(0)] \\ & + \frac{1}{1,209,600n^8}\,[f^{(7)}(1) - f^{(7)}(0)] \\ & - \frac{1}{47,900,160n^{10}}\,[f^{(9)}(1) - f^{(9)}(0)]\end{aligned} \tag{5.4.16}$$

as $n \to \infty$.

Example 5.4.3 We use the formula (5.4.16) to obtain an approximation of the integral

$$\begin{aligned} J_0(2) &= \frac{1}{\pi}\int_0^{\pi} \cos[2\sin\theta]d\theta \\ &= \int_0^1 \cos[2\sin \pi\, x]dx,. \end{aligned} \tag{5.4.17}$$

In this case, we easily prove by induction that $(\cos[2\sin\pi x])^{(2k-1)} = 0$ for $x = 0$ and $x = 1$, and for every positive integer k. At first glance, (5.4.16) leads us to suspect that the integral (5.4.17) is equal to its trapezoidal sum, for $n = 1, 2, 3, \ldots$. This is not the case. Equation (5.4.14) merely tells us that as $n \to \infty$, the error, $J_0(x) - T_n(\cos[2\sin\pi x])$ approaches zero faster than any power of $1/n$. The results of the computations are given in Table 5.4.2.

Table 5.4.2: The approximation of $J_0(2)$.

n	$T_n(\cos[\sin\pi x])$	$J_0(2)$
2	.29192	
3	.22630	.22389079
4	.223935	
6	.22389079	
8	.22389078	
12	.22389078	

The Euler-Maclaurin formula (5.4.14) is sometimes written in the form

$$\int_0^{nh} f(t)dt = T_h(f) - C(2m, nh) + R(2m, nh) \tag{5.4.18}$$

where

$$\begin{aligned} T_h(f) &= h\left[\frac{1}{2}f(0) + f(h) + \cdots + f((n-1)h) + \frac{1}{2}f(nh)\right] \\ C(2m, nh) &= \sum_{k=1}^{m} h^{2k}P_{2k}(0)[f^{(2k-1)}(nh) - f^{(2k-1)}(0)] \\ R(2m, nh) &= h^{2m+1}\int_0^{nh} P_{2m}(t/h)f^{(2m)}(t)dt\,, \end{aligned} \tag{5.4.19}$$

this formula being valid, for example, if $f \in C^{(2m)}[0, nh]$.

If we let $n \to \infty$ in (5.4.18), we arrive at:

Theorem 5.4.4 *Let* $\int_0^\infty |f(t)|dt$ *exist, and let* $\int_0^\infty |f^{(2m)}(t)|dt < \infty$. *Then*

$$\int_0^\infty f(t)dt = h\left[\frac{1}{2}f(0) + f(h) + f(2h) + \cdots\right]$$

$$+\sum_{k=1}^{m} h^{2k} P_{2k}(0) f^{(2k-1)}(0) \qquad (5.4.20)$$
$$+h^{2m+1} \int_0^\infty P_{2m}(t/h) f^{(2m)}(t)\,dt,.$$

Corollary 5.4.5 *Let $\int_0^\infty |f(t)|dt$ exist, and let $\int_0^\infty |f^{(2m)}(t)|dt < \infty$ for $m = 1, 2, 3, \ldots$. Then*

$$\begin{aligned}\int_0^\infty f(t)dt \quad &\sim \quad h\left[\frac{1}{2} f(0) + f(h) + f(2h) + \cdots\right] \\ &\quad + \sum_{k=1}^{m} h^{2k} P_{2k}(0) f^{2k-1}(0)\end{aligned} \qquad (5.4.21)$$

as $h \to 0$.

Let us next replace $f(t)$ in Theorem 5.4.4 by $g(t+a)$. Letting $a \to -\infty$, we arrive at:

Theorem 5.4.6 *Let $\int_{-\infty}^\infty |f(t)|dt$ exist, and let $\int_{-\infty}^\infty |f^{2m}(t)|dt < \infty$. Then*

$$\begin{aligned}\int_{-\infty}^\infty f(t)dt \quad &= \quad h \sum_{k=-\infty}^{\infty} f(kh) \\ &\quad + h^{2m+1} \int_{-\infty}^\infty P_{2m}\left(\frac{t}{h}\right) f^{(2m)}(t)\,dt\,.\end{aligned} \qquad (5.4.22)$$

Corollary 5.4.7 *Let $\int_{-\infty}^\infty |f(t)|dt$ exist, and let $\int_{-\infty}^\infty |f^{(2m)}(t)|dt < \infty$ for $m = 1, 2, 3, \ldots$. Then*

$$\int_{-\infty}^\infty f(t)dt - h \sum_{k=-\infty}^{\infty} f(kh) = 0(h^\alpha) \qquad (5.4.23)$$

as $h \to 0$ where $\alpha > 0$ is arbitrary.

Example 2: The result of Corollary 5.4.5 may be used not only to approximate integrals, but also to evaluate some slowly convergent series. For example, to evaluate

$$S = \sum_{n=0}^{\infty} (1/(n+1)^2)$$

correct to 8 decimals we would need to sum about 10,000 terms of the series. If we set $h = 1$ in (5.4.21), we get

$$\begin{aligned} S = \sum_{n=0}^{\infty} \frac{1}{(1+n)^2} &\cong \int_0^{\infty} \frac{dx}{(1+x)^2} + \frac{1}{2} + \sum_{k=1}^{m} (-1)^{k-1} B_{2k} \\ &= \frac{3}{2} + \sum_{k=1}^{m} (-1)^{k-1} B_{2k} \end{aligned} \qquad (5.4.24)$$

since $f^{2k-1}(0) = (-1)^k (2k)!$. The error between the true result ($S = \pi^2/6$) and the approximation as a function of m on the extreme right of (5.4.24) is given in Table 5.4.3.

Table 5.4.3: The error of the approximation (??? 5.4.24)

m	0	1	2	3	4	5
Error	.145	-.022	.012	-.012	.021	-.055

Let us next approximate

$$S_1 = \sum_{n=0}^{\infty} 1/(10+n)^2 .$$

We obtain

$$S_1 = \sum_{n=0}^{\infty} \frac{1}{(10+n)^2} \cong \int_0^{\infty} \frac{dx}{(10+x)^2} + \frac{1}{2} \cdot \frac{1}{10^2} + \sum_{k=1}^{m} \frac{B_{2k}}{10^{2k+1}} . \qquad (5.4.25)$$

With $m = 2$, the right of (5.4.25) yields

$$S_1 \cong \frac{1}{10} + \frac{1}{200} + \frac{1}{6} \cdot \frac{1}{10^3} - \frac{1}{30 \cdot 10^5} \cong \cdot 1051663333 .$$

We now add this result to the directly calculated sum

$$\sum_{n=1}^{9} \frac{1}{n^2} \cong 1.5397677311$$

to get

$$S = 1.6449340644$$

which is correct to 8 decimals.

This result illustrates very well the asymptotic nature of the Euler-Maclaurin formula. Although the series

$$\sigma = \sum_{k=1}^{\infty} \frac{B_{2k}}{a^{2k+1}}$$

diverges for every $a > 0$ when a is large, the series begins to converge very rapidly; for the case of (5.4.25), it may be shown that the error upon truncating σ after m terms is less in magnitude than the magnitude of the first neglected term.

Example 3:

$$I = \int_1^{n+1} \log t \, dt = \int_0^n \log(1+t) dt \, .$$

For this case,

$$\frac{d^{2k-1}}{dt^{2k-1}} (\log(t+1)) = \frac{(2k-1)\,!}{(t+1)^{2k-1}} \, , \quad k \geq 1 \, .$$

All of these derivatives have the same sign throughout the interval of integration; this fact enables us to conclude that if we use $h = 1$ in (5.4.18) then

$$\begin{aligned} I &= \log 2 + \log 3 + \cdots + \log n + \frac{1}{2} \log(n+1) \\ &\quad - \sum_{k=1}^{m} P_{2k}(0) \left[\frac{1}{(n+1)^{2k-1}} - 1 \right] (2k-1)\,! \, , \end{aligned}$$

the error is less than the first neglected term. Also, I can be explicitly evaluated to yield $I = (n+1)\log(n+1) - n$. Hence we obtain using (5.4.19)

$$\log((n+1)\,!) = \left(n + \frac{3}{2}\right) \cdot \log(n+1) - n - C(2m, n) + R(2m, n)$$

where

$$|R(2m, n)| < (2m-2)\,! \, |P_{2m}(0)| \left[1 - \frac{1}{n} 2m - 1 \right] \, .$$

Example 4: The two integrals

$$\int_0^{\infty} e^{-t} \cos xt \, dt \quad \text{and} \quad \int_0^{\infty} e^{-t} \sin xt \, dt$$

can be handled simultaneously by means of

$$I(x) = \int_0^\infty e^{-t(1-ix)} dt \, .$$

For the integrand in this integral,

$$\frac{d^k}{dt^k}\left(e^{-t(1-ix)}\right) = (-1)^k (1-ix)^k e^{-t(1-ix)}$$

and so

$$\left| \frac{d^k}{dt^k} e^{-t(1-ix)} \right| \le (1+x^2)^{k/2} e^{-t} \, .$$

Consequently, using (5.4.20),

$$\begin{aligned} I(x) &= h\left[\frac{1}{2} + e^{-h(1-ix)} + e^{-2h(1-ix)} + \cdots\right] \\ &\quad - \sum_{k=1}^{m} h^{2k} P_{2k}(0)(1-ix)^{2k-1} + R(2m,\infty) \end{aligned}$$

where

$$R(2m,\infty) = h^{2m+1} \int_0^\infty P_{2m}(t/h)(1-ix)^{2m} e^{-t(1-ix)} dt$$

so that

$$|R(2m,\infty)| \le h^{2m+1} |P_{2m}(0)| (1+x^2)^m \, .$$

For fixed m and x, $R(2m,\infty)$ can thus be chosen as small as we please, by taking h sufficiently small.

Example 5:

$$I = \int_{-\infty}^{\infty} e^{-t^2} dt$$

The results of Corollary 5.4.7 apply to this integral, and we may therefore expect the approximation

$$I \cong h \sum_{k=-\infty}^{\infty} e^{-k^2 h^2}$$

to be quite accurate. That this is indeed the case, is illustrated in Table 5.4.4.

Table 5.4.4: $\int_{-\infty}^{\infty} exp(-t^2)\, dt = 1.77245385$

h	$I \simeq h \sum_{-\infty}^{\infty} e^{k^2 h^2}$
1	1.77263720
1/2	1.77245377

For this problem we can get an estimate on the rate of convergence, using the identity

$$I(x) = \int_{-\infty}^{\infty} e^{-t^2} \cos xt\, dt = (2\pi)^{1/2} e^{-x^2/4}$$

which yields

$$\left(\frac{d}{dx}\right)^{2m} I(x) = \int_{-\infty}^{\infty} e^{-t^2} t^{2m} \cos(xt) dt = (2\pi)^{1/2} \frac{d^{2m}}{dx^{2m}} \left(e^{-x^2/4}\right) . \quad (5.4.26)$$

Thus, using (5.4.22), the error with $m = 1$ is

$$\epsilon = h^3 \int_{-\infty}^{\infty} P_2(t/h)[4t^2 - 2] e^{-t^2} dt .$$

Taking only the first term in the Fourier series of P_2 in (5.4.7), we get

$$\begin{aligned} \epsilon &\cong h \int_{-\infty}^{\infty} \frac{2\cos(2\pi t/h)}{4\pi^2} [4t^2 - 2] e^{-t^2} dt \\ &= \frac{2(2\pi)^{1/2}}{\pi^2} h(\pi^2 - h^2) e^{-\pi^2/h^2} \cong 5h\, e^{-\pi^2/h^2} , \end{aligned}$$

where we have used (5.4.26) to evaluate the integral. Hence $\epsilon \cong 2 \cdot 5 \times 10^{-4}$ with $h = 1$, while $\epsilon \cong 3 \times 10^{-17}$ with $h = 1/2$.

Problems

5.4.1 Derive the series (5.4.6).

5.4.2 Define the Bernoulli polynomials $B_n(x)$ by means of the generating function

$$\frac{z e^{xz}}{e^z - 1} = \sum_{n=0}^{\infty} \frac{B_n(x)}{n!} z^n .$$

Differentiate each side to conclude that

$$\frac{z^2 e^{xz}}{e^z - 1} = \sum_{n=1}^{\infty} B_n(x)\frac{z^n}{n!} = \sum_{n=1}^{\infty} n\, B_{n-1}(x)\frac{z^n}{n!},$$

i.e., that $B_n(x) = n\, B_{n-1}(x)$.

5.4.3 Define $B_n = B_n(0)$, and conclude that

$$B_n(x) = B_n + n\int_0^x B_{n-1}(t)dt\ ,\quad n = 1, 2, 3, \ldots .$$

5.4.4 Verify (5.4.10).

5.4.5 Derive the equation (5.4.14), using (5.4.13).

5.4.6 Use (5.4.21) to evaluate $\sum\limits_{n=1}^{\infty} 1/n^3$ correct to eight decimals.

5.4.7 Evaluate $\int_0^{\infty} e^{-x^2}\cos 2x\, dx$ correct to five significant figures.

5.4.8 Derive the formula

$$\begin{aligned} h\int_0^1 f(a+\zeta h)d\zeta - hf\left(a+\frac{1}{2}h\right) &= \sum_{r=1}^{m} h^{2r}P_{2r}\left(\frac{1}{2}\right)[f^{(2r-1)}(a+h) - f^{(2r-1)}(a)] \\ &\quad + h^{2m+1}\int_0^{nh} P_{2m}\left(\zeta - \frac{1}{2}\right) f^{(2m)}(a+\zeta h)d\zeta \end{aligned}$$

which is valid, for example, if $f \in C^{(2m)}[a, a+h]$.

5.4.9 Use the results of Problem 5.4.8 to deduce the formula

$$\begin{aligned} h\int_0^{nh} f(a &+\zeta h)d\zeta - h\textstyle\sum_{k=1}^{n} f\left(a + \frac{2k-1}{2}h\right) \\ &= \textstyle\sum_{r=1}^{m} h^{2r}P_{2r}\left(\frac{1}{2}\right)[f^{(2r-1)}(a+nh) - f^{(2r-1)}(a)] \\ &\quad + h^{2m+1}\textstyle\int_0^{nh} P_{2m}\left(\zeta - \frac{1}{2}\right) f^{(2m)}(a+\zeta h)d\zeta\,. \end{aligned}$$

5.4.10 Use the results of Problem 5.4.9 to deduce that if $f \in C^{(m)}[0,1]$ for every $m = 1, 2, 3, \ldots$, then

$$\begin{aligned}\int_0^1 f(x)dx &= M_n(f) + \frac{1}{24n^2}[f'(1) - f'(0)] - \frac{7}{5760\, n^4}[f^{(3)}(1) - f^{(3)}(0)] \\ &\quad + \frac{31}{967,680\, n^6}[f^{(5)}(1) - f^{(5)}(0)]\end{aligned}$$

$$-\frac{127}{154,828,800\, n^8}[f^{(7)}(1) - f^{(7)}(0)] + 0(n^{-10})$$

as $n \to \infty$, where $M_n(f)$ is defined in (5.3.7).

5.4.11 Combine (5.4.26) and the result of Problem 5.4.8 that if

$$\int_0^\infty |f^{(2m)}(t)|dt < \infty$$

for $m = 1, 2, 3, \ldots$ then

$$\begin{aligned}\int_0^\infty f(t)dt - \sum_{n=1}^\infty f\left(\frac{2n-1}{2}h\right) &= -\frac{h^2}{24} f'(0) + \frac{7h^4}{5760} f^{(3)}(0) \\ &\quad - \frac{31}{967,680} f^{(5)}(0) + \frac{127\, h^8}{154,828,800} f^{(7)}(0) + 0(h^{10})\end{aligned}$$

as $h \to 0$.

5.4.12 $*$ Show that $B_k\left(\frac{1}{2}\right) = 2(2^{-k} - 1)B_k$.

5.5 The Romberg Algorithm

In practice it is possible to achieve only limited accuracy by the trapezoidal and midordinate formulas, because of the large number of points that are required and because of roundoff error. The Romberg method attempts to avoid this problem by producing a more rapidly convergent expansion of $\int_0^1 f(x)dx$. Starting from (5.4.16) we see that

$$\int_0^1 f(x)dx \sim T_n(f) + \frac{a_1}{n^2} + \frac{a_2}{n^4} + \frac{a_3}{n^6} + \cdots \qquad (5.5.1)$$

where the a's depend on f but not on n. If we replace n by $2n$ in this relation, then

$$\int_0^1 f(x)dx \sim T_{2n}(f) + \frac{a_1}{4n^2} + \frac{a_2}{16n^4} + \frac{a_3}{64n^6} + \cdots . \tag{5.5.2}$$

We multiply (5.5.2) by 2^2, subtract (5.5.1), and divide the result by $2^2 - 1$, to get

$$\int_0^1 f(x)dx \sim \frac{2^2 T_{2n}(f) - T_n(f)}{2^2 - 1} + \frac{1}{2^2-1}\left[\left(\frac{2^2}{2^4} - 1\right)\frac{a_2}{n^4} + \cdots\right] . \tag{5.5.3}$$

If we use the notation $T_n^{(1)} = T_n(f)$, and

$$T_{2n}^{(2)} = \frac{2^2 T_{2n}^{(1)} - T_n^{(1)}}{2^2 - 1} \tag{5.5.4}$$

we see that, while

$$\int_0^1 f(x)dx = T_n^{(1)} + 0\left(\frac{1}{n^2}\right) \ , \quad n \to \infty \, , \tag{5.5.5}$$

$$\int_0^1 f(x)dx = T_{2n}^{(2)} + 0\left(\frac{1}{n^4}\right) \ , \quad n \to \infty \, . \tag{5.5.6}$$

In general, if we define $T_m^{(j+1)}$ by

$$T_{2^k n}^{(j+1)} = \frac{2^{2j} T_{2^k n}^{(j)} - T_{2^{k-1} n}^{(j)}}{2^{2j} - 1} \tag{5.5.7}$$

for $j = 1, 2, 3, \ldots$, and $k = j,\ j+1, j+2, \ldots$, then it may be shown that

$$\int_0^1 f(x)dx = T_{2^k n}^{(j+1)} + 0\left(\frac{1}{n^{2j+2}}\right) \ , \quad n \to \infty \, . \tag{5.5.8}$$

The following table illustrates the method of tabulating the sequence of numbers.

It may be shown that in theory, each of the columns in Table 5.5.1 converges to $\int_0^1 f(x)dx$, the rate of convergence of the j'th column being $0(n^{-2j})$ as $n \to \infty$.

In order to get the j'th column in Table 5.5.1, we have of course assumed that $f^{(2j-1)}(x)$ exists on the interval $[0, 1]$. This does not hold for every integer j, for example, when $f(x) = x^a$, and a is not an integer. Also, the columns of the Romberg table may appear to converge initially—to the wrong value.

Table 5.5.1: The Romberg Table

$T_n^{(1)}$				
$T_{2n}^{(1)}$	$T_{2n}^{(2)}$			
$T_{2^2n}^{(1)}$	$T_{2^2n}^{(2)}$	$T_{2^2n}^{(3)}$		
$T_{2^3n}^{(1)}$	$T_{2^3n}^{(2)}$	$T_{2^3n}^{(3)}$	$T_{2^3n}^{(4)}$	
$T_{2^4n}^{(1)}$	$T_{2^4n}^{(2)}$	$T_{2^4n}^{(3)}$	$T_{2^4n}^{(4)}$	$T_{2^4n}^{(5)}$

Example 5.5.1 Let us evaluate

$$\log 3 = \int_0^1 \frac{2dx}{2x+1} \cong 1.098612$$

by use of the Romberg algorithm. The results we obtain are given in Table 5.5.2.

Table 5.5.2: The Romberg Algorithm

j	$T_{2^j}^{(1)}$	$T_{2^j}^{(2)}$	$T_{2^j}^{(3)}$	$T_{2^j}^{(4)}$
0	1.333333			
1	1.166667	1.111111		
2	1.116667	1.100000	1.099259	
3	1.103211	1.098725	1.098641	1.098631

Problems

5.5.1 Explain why the Romberg method fails for the case of

$$\int_0^1 x \log x dx \quad \text{or} \quad \int_0^1 (x^{1/3} + x^{1/4}) dx$$

5.5.2 How is $T_{2^k n}^{(2)}$ related to Simpson's rule (see(5.3.12))?

5.5.3 Derive the Romberg algorithm using the midordinate, rather than the trapezoid rule. (Solution: Simply replace the T's with M's in the equations of this section. Why?)

5.5.4 Apply the Romberg method to approximate

(a) $\int_0^1 x^{1/2}dx$

(b) $\int_0^1 \log(x)dx$

(For the case of (b), use $M_{2^k n}^{(j+1)}$ procedure of Problem 5.5.3 as well as the $T_{2^k n}^{(j+1)}$ procedure of the chapter.)

5.6 Gaussian Quadrature

Let $w(x) > 0$ on the interval (a, b), and let us introduce the inner product notation

$$(f, g) = \int_a^b w(x)f(x)g(x)dx \tag{5.6.1}$$

where f and g are continuous functions on (a, b). We assume that the numbers

$$\mu_k = (x^k, 1) = \int_a^b w(x)x^k dx \tag{5.6.2}$$

are finite for every integer $k \geq 0$. We can then use the Gram-Schmidt process to construct a sequence of polynomials $\{\psi_k\}_{k=0}^{\infty}$ that are orthonormal over (a, b) with respect to $w(x)$; that is,

$$(\psi_k, \psi_\ell) \equiv \int_a^b w(x)\psi_k(x)\psi_\ell(x)dx = \delta_{k\ell} = \begin{cases} 1 & k = \ell \\ 0 & k \neq \ell \end{cases}. \tag{5.6.3}$$

In particular, we may assume that

$$\psi_n(x) = k_n x^n + s_n x^{n-1} + \pi_{n-2}(x) \tag{5.6.4}$$

where $k_n > 0$, and where $\pi_{n-2}(x)$ is a polynomial of degree $n - 2$ in x.

The Gram-Schmidt construction is based on the same principles as in Chapter 2 and proceeds as follows: Define

$$\begin{aligned} \psi_0(x) &= (1, 1)^{-1/2} \\ \psi_n(x) &= (\theta_n, \theta_n)^{-1/2}\theta_n(x) \end{aligned} \tag{5.6.5}$$

where

$$\theta_n(x) = x^n - \sum_{j=0}^{n-1} (x^n, \psi_j)\psi_j(x) \tag{5.6.6}$$

then the $\{\psi_n\}_0^\infty$ satisfy (5.6.3) (Problem 5.5.1). It can be shown that the n zeros of $\psi_n(x)$ are real, distinct and lie within the interval (a, b) (Problem 5.5.3). This fact plays a role in the quadrature formula based on the $\{\psi_n\}_{n=0}^\infty$. If we multiply the Lagrange polynomial that interpolates a function f at the zeros x_j of ψ_n by $w(x)$ and integrate over (a, b), we obtain

$$\begin{aligned}\int_a^b w(x)f(x)dx &\cong \int_a^b w(x)\sum_{j=1}^n f(x_j)\left[\frac{\psi_n(x)}{(x-x_j)\psi_n'(x_j)}\right]dx \\ &= \sum_{j=1}^n w_j f(x_j)\end{aligned} \tag{5.6.7}$$

where

$$w_j = \int_a^b w(x)\frac{\psi_n(x)}{(x-x_j)\psi_n'(x_j)}dx\,. \tag{5.6.8}$$

The approximation (5.6.7) with w_j chosen as in (5.6.8) is known as Gaussian quadrature.

We now derive some properties of Gaussian quadrature.

Lemma 5.6.1 *$w_j > 0$, $j = 1, 2, \ldots, n$.*

Proof: We multiply the integrand in (5.6.7) by

$$1 = \sum_{k=1}^n \frac{\psi_n(x)}{(x-x_k)}\,\psi_n'(x_k) \tag{5.6.9}$$

to obtain

$$\begin{aligned} w_j &= \int_a^b \left(\sum_{k=1}^n \frac{\psi_n(x)}{(x-x_k)\psi_n'(x_k)}\right)\frac{\psi_n(x)}{(x-x_j)\psi_n'(x_j)} \\ &\equiv \left(\sum_{k=1}^n \frac{\psi_n(x)}{(x-x_k)\psi_n'(x_k)}\,,\quad \frac{\psi_n(x)}{(x-x_j)\psi_n'(x_j)}\right) \\ &= \left(\frac{\psi_n(x)}{(x-x_j)\psi_n'(x_j)}\,,\quad \frac{\psi_n(x)}{(x-x_j)\psi_n'(x_j)}\right) \end{aligned} \tag{5.6.10}$$

$$
+ \sum_{\substack{k=1 \\ k \neq j}}^{n} \left(\psi_n(x) \; , \quad \frac{\psi_n(x)}{(x-x_j)(x-x_k)\psi_n'(x_j)\psi_n'(x_k)} \right)
$$

$$
= \left(\frac{\psi_n(x)}{(x-x_j)\psi_n'(x_j)} \; , \quad \frac{\psi_n(x)}{(x-x_j)\psi_n'(x_j)} \right)
$$

since each of the polynomials

$$
P_{jk}(x) = \frac{\psi_n(x)}{(x-x_j)(x-x_k)\psi'(x_j)\psi'(x_k)} \tag{5.6.11}
$$

is of degree less than n, which implies (c.f. Problem 5.6.2) that $(\psi_n, P_{jk}) = 0$. On the other hand, the term on the extreme right of (5.6.10) is positive, and so $w_j > 0$.

Lemma 5.6.2 *Let $P_{2n-1}(x)$ be any polynomial of degree $2n-1$ in x. Then there are polynomials $q_{n-1}(x)$ and $r_{n-1}(x)$, both of degree $n-j$ in x, such that*

$$
P_{2n-1}(x) = \psi_n(x) q_{n-1}(x) + r_{n-1}(x) \,. \tag{5.6.12}
$$

Proof: This is left as a problem (Problem 5.6.5).

Lemma 5.6.3 *The formula*

$$
\int_a^b w(x) f(x) dx = \sum_{j=1}^{n} w_j f(x_j) \tag{5.6.13}
$$

holds whenever $f(x)$ is any polynomial of degree $2n-1$ in x.

Proof: If $r_{n-1}(x)$ is any polynomial of degree $n-1$ in x, then (c.f. Chapter 2)

$$
r_{n-1}(x) = \sum_{j=1}^{n} \frac{\psi_n(x) r_{n-1}(x_j)}{(x-x_j) r_{n-1}^{1}(x_j)} \,. \tag{5.6.14}
$$

It follows therefore from (5.6.7) that

$$
\int_a^b w(x) r_{n-1}(x) dx = \sum_{j=1}^{n} w_j r_{n-1}(x_j) \,. \tag{5.6.15}
$$

On the other hand, if $P_{2n-1}(x)$ is an arbitrary polynomial of degree $2n-1$ in x, then using Lemma 5.6.2, we get

$$\begin{aligned}\int_a^b w(x)P_{2n-1}(x)dx &= \int_a^b w(x)\psi_n(x)q_{n-1}(x)dx \\ &\quad + \int_a^b w(x)r_{n-1}(x)dx \\ &= \int_a^b w(x)r_{n-1}(x)dx\end{aligned} \tag{5.6.16}$$

since $(\psi_n, q_{n-1}) = 0$. We similarly note that

$$\begin{aligned}\sum_{j=1}^{n} w_j P_{2n-1}(x_j) &= \textstyle\sum_{j=1}^{n} w_j[\psi_n(x_j)q_{n-1}(x_j) + r_{n-1}(x_j)) \\ &= \textstyle\sum_{j=1}^{n} w_j r_{n-1}(x_j)\end{aligned} \tag{5.6.17}$$

since $\psi_n(x_j) = 0$ for $j = 1, 2, \ldots, n$. We now combine (5.6.15), (5.6.16) and (5.6.17), to arrive at the completion of the proof of Lemma 5.6.3.

Theorem 5.6.4 *Let f be any function such that $(f, 1) < \infty$, and such that $f^{(2n)}(x)$ exists on (a, b). Then*

$$\int_a^b w(x)f(x)dx = \sum_{j=1}^{n} w_j f(x_j) + \frac{f^{(2n)}(\zeta)}{(2n)!\,k_n^2} \tag{5.6.18}$$

where $\zeta \in (a, b)$, and k_n is defined in (5.5.4).

Proof: We recall (Chapter 4) the Lagrange-Hermite interpolation polynomial $P_{2n-1}(x)$ of degree $2n-1$ in x that satisfies

$$\begin{aligned}P_{2n-1}(x_j) &= f(x_j) \\ P_{2n-1}(x_j) &= f'(x_j)\end{aligned} \tag{5.6.19}$$

for $j = 1, 2, \ldots, n$, and also

$$f(x) - P_{2n-1}(x) = \frac{f^{(2n)}(\zeta)}{(2n)!\,k_n^2}\ \psi_n^2(x)\,, \tag{5.6.20}$$

where $\zeta = \zeta(x) \in (a, b)$ if $x \in [a, b]$. Upon setting

$$\epsilon(g) = \int_a^b w(x)g(x)dx - \sum_{j=1}^{n} w_j g(x_j) \tag{5.6.21}$$

and noting that $\epsilon(P_{2n-1}) = 0$, by Lemma 5.6.3, we obtain

$$\epsilon(f) = \epsilon(f) - \epsilon(P_{2n-1}) = \epsilon(f - P_{2n-1}) = \epsilon\left(\frac{f^{(2n)}(\zeta(x))}{(2n)!\,k_n^2}\right)\ \psi_n^2(x)\,. \tag{5.6.22}$$

Moreover, since $(\psi_n, \psi_n) = 1$ for $j = 1, 2, \ldots, n$, it follows that

$$\begin{aligned} \epsilon(f) &= \int_a^b w(x)\frac{f^{(2n)}(\zeta(x))}{(2n)!\,k_n^2}\ \psi_n^2(x)dx \\ &= \frac{f^{(2n)}(\zeta)}{(2n)!\,k_n^2}\int_a^b w(x)\psi_n^2(x)dx \qquad (5.6.23) \\ &= \frac{f^{(2n)}(\zeta)}{(2n)!\,k_n^2}\,,\ \zeta \in (a, b) \end{aligned}$$

using the result $(\psi_n, \psi_n) = 1$. This completes the proof of Theorem 5.6.4??.

When constructing quadrature formulas, it suffices by Sec. 5.3 to restrict ourselves to the intervals $(0, 1)$ or $(-1, 1)$ in the case when a and b are finite. For the case of the integral $\int_a^\infty f(y)dy$, we set $y = a + x$, and thus reduce to another standard interval $(0, \infty)$, while if $a = -\infty$ and $b = \infty$, we leave the interval unchanged.

Example 5.6.5 **(Gauss-Legendre Quadrature)** Here $w(x) = 1$, $a = -1$, $b = 1$. The orthogonal polynomials are the Legendre polynomials. The zeros $x_j^{(n)}$ and the corresponding weights $w_j^{(n)}$ are given in Table 5.6.1. The explicit expression for n-point Gauss-Legendre quadrature with error is

$$\int_{-1}^{1} f(x)dx = \sum_{j=1}^{n} w_j^{(n)} f(x_j^{(n)}) + \frac{2^{(2n+1)}(n!)^4 f^{(2n)}(\zeta)}{(2n+1)[(2n)!]^3} \tag{5.6.24}$$

where $\zeta \in (-1, 1)$.

Table 5.6.1: Abscissas and Weights for Gaussian-Legendre Integration

$x_j^{(n)}$	$w_j^{(n)}$
$n=2$	
.577350269	1.000000000
$n=3$	
.774596669	.555555556
.000000000	.888888889
.861136311	.347854845
.339981043	.652145155
$n=5$	
.906179846	.236926895
.538469310	.478628670
.000000000	.568888899
$n=6$	
.932469514	.171324452
.661209386	.360761573
.238619186	.467913934

Example 5.6.6 **(Gauss-Chebyshev Quadrature)** Here $a=-1$, $b=1$, and $w(x)=(1-x^2)^{-1/2}$. The orthogonal polynomials are the Chebyshev polynomials, $T_n(x)=\cos n\theta$, where $x=\cos\theta$. The zeros $x^{(n)}$ and the weights $w_j^{(n)}$ can be explicitly expressed:

$$\begin{aligned} x_j^{(n)} &= \cos\left[\tfrac{(2j-1)\pi}{2n}\right] \\ w_k^{(n)} &= \tfrac{\pi}{n}\,. \end{aligned} \tag{5.6.25}$$

Thus it may be shown that if $f\in C^{(2n)}[-1,1]$,

$$\int_{-1}^{1}\frac{f(x)}{\sqrt{1-x^2}}\,dx=\frac{\pi}{n}\sum_{j=1}^{n} f\left(\cos\left[\frac{2j-1}{2n}\,\pi\right]\right)+\frac{\pi}{2^{2n-1}(2n)!}\,f^{(2n)}(\zeta) \tag{5.6.26}$$

where $\zeta\in(-1,1)$. This is the Gauss-Chebyshev quadrature based on the Chebyshev polynomials of the first kind $T_n(x)=\cos(n\theta)$, $\cos\theta=x$.

Example 5.6.7 **(Gauss-Laguerre Quadrature)** In this case $a=0$, $b=\infty$, and $w(x)=e^{-x}$. The orthogonal polynomials are the Laguerre polynomials. The zeros $x_j^{(n)}$ and the corresponding weights $w_j^{(n)}$ are given in Table 5.6.2 for several values of n. The explicit formula for Gauss-Laguerre quadrature with error is

$$\int_0^\infty e^{-x} f(x)dx = \sum_{j=1}^n w_j^{(n)} f(x_j^{(n)}) + \frac{(n\,!)^2}{(2n)\,!} f^{(2n)}(\zeta)\,, \qquad (5.6.27)$$

where $\zeta \in (0, \infty)$.

Example 5.6.8 (Gauss-Hermite Quadrature) Here $a = -\infty$, $b = \infty$, and $w(x) = e^{-x^2}$. The orthogonal polynomials are the Hermite polynomials. The explicit form of Gauss-Hermite quadrature with error is

$$\int_{-\infty}^\infty e^{-x^2} f(x)dx = \sum_{j=1}^n w_j^{(n)} f(x_j^{(n)}) + \frac{\sqrt{\pi}\; n\,!}{2^n(2n)\,!} f^{(2n)}(\zeta) \qquad (5.6.28)$$

where $\zeta \in (-\infty, \infty)$. The zeros $x_j^{(n)}$ and the corresponding weights $w_j^{(n)}$ are given in Table 5.6.3 for the first few values of n.

Tables exist for a number of different types of quadrature formulas. We refer the reader to Davis and Robinowitz [1], Strond and Secrest [2], and to the National Bureau of Standards Handbook of Mathematical Functions [3] for these. Recently, there has been considerable emphasis on the replacement of tables by efficient algorithms that generate the zeros and weights of Gaussian quadrature; here we refer the reader to Gautschi [4].

Example 6: Evaluate

$$I = \int_0^1 e^y dy\,.$$

If we use the trapezoidal formula, we obtain

$$I = \frac{1}{n}\left[\frac{1}{2} + e^{1/n} + e^{2/n} + \cdots + e^{(n-1)/n} + \frac{1}{2}e\right] + \epsilon$$

where $\epsilon = -e^\zeta/(12n^2)$, for some $\zeta \in (0, 1)$. Thus the magnitude of the error is at least $1/(12n^2)$.

Transforming the integral to $(-1, 1)$, we also have

$$I = \frac{1}{2}e^{1/2}\int_{-1}^1 e^{x/2}dx\,.$$

Using Gauss-Legendre quadrature to evaluate the integral, we get

$$I = \frac{1}{2}e^{1/2}\sum_{j=1}^n w_j^{(n)} e^{x_j^{(n)}/2} + \epsilon(e^{x/2})$$

Table 5.6.2: Abscissas and Weights for Gaussian–Laguerre Integration

$x_j^{(n)}$	$w_j^{(n)}$
$n = 2$	
0.585786437	0.853553390
(1)0.341421356	0.146446609
$n = 3$	
0.415774556	0.711093009
(1)0.229428036	0.278517733
(1)0.628994508	(-1)0.103892565
$n = 4$	
0.322547689	0.603154104
(1)0.174576110	0.357418592
(1)0.453662029	(-1)0.388879085
(1)0.939507091	(-3)0.539294705
$n = 5$	
0.263560319	0.521755610
(1)0.141340305	0.398666811
(1)0.359642577	(-1)0.759424496
(1)0.708581000	(-2)0.361175867
(2)0.126408008	(-4)0.233699723
$n = 6$	
0.222846604	0.458964673
(1)0.118893210	0.417000830
(1)0.299273632	0.113373382
(1)0.577514356	(-1)0.103991974
(1)0.983746741	(-3)0.261017202
(2)0.159828739	(-6)0.898547906

$(d)0.a_1a_2 = .a_1a_2 \times 10^d$

Table 5.6.3: Abscissas and Weights for Gaussian–Hermite Integration

$x_j^{(n)}$		$w_j^{(n)}$
	$n = 2$	
0.707106781		0.886226925
	$n = 3$	
(1)0.122474487		0.295408975
0.000000000		(1)0.118163590
	$n = 4$	
(1)0.165068012		(-1)0.813128354
0.524647623		0.804914090
	$n = 5$	
(1)0.202018287		(-1)0.199532420
0.958572464		0.393619323
0.000000000		0.945308720
	$n = 6$	
(1)0.235060497		(-2)0.453000990
(1)0.133584907		0.157067320
0.436077411		0.724629595

$(d)0.a_1a_2 = .a_1a_2 \times 10^d$

where, using (**??**)

$$\epsilon(e^{x/2}) = \frac{1}{2}\, e^{1/2} \cdot \frac{2^{2n+1}(n\,!\,)^4}{(2n+1)[(2n)\,!\,]^3} \left(\frac{d^{2n}}{dx^{2n}}\,(e^{x/2}) \right) \Big|_{x=\zeta},$$

and where $\zeta \in (-1, 1)$. Since $(e^{x/2})^{(2n)} = (1/2)^{2n} e^{x/2}$ we find that the error of Gaussian quadrature is

$$\begin{aligned} \epsilon(e^{x/2}) &= \frac{e^{(\xi+1)/2}(n\,!\,)^4}{(2n+1)[(2n)\,!\,]^3} \\ &\le e \left(\frac{2\pi}{n}\right)^{1/2} \left(\frac{e}{8n}\right)^{2n} \end{aligned}$$

where Sterling's formula is used to obtain the inequality in (5.6.24). A comparison of the error bounds are listed in Table 5.6.4.

The above example illustrates the rapid convergence of Gaussian quadrature when applied to a suitable integrand. Rapid convergence occurs for

Table 5.6.4: Error Bounds for Example ??

n	Lower Bound for Trapezoidal Error	Upper Bound for Gauss-Legendre Error
2	2.1×10^{-2}	4.0×10^{-3}
5	3.3×10^{-3}	6.4×10^{-12}
10	8.3×10^{-4}	9.1×10^{-30}

those functions whose $2n$'th derivative exists for every positive integer n, and grows slowly as a function of n. The function $e^{x/2}$ is of this type.

An integral

$$I = \int_a^b F(y)dy \tag{5.6.29}$$

can be effectively approximated by Gaussian quadrature if the following conditions are met.

(i) It is possible to write

$$I = \int_a^b w(x)f(x)dx \tag{5.6.30}$$

where $w(x) > 0$ on (a, b), and where the maximum value of the $2n$'th derivative of f on $[a, b]$ grows slowly as a function of n. This condition is met, for example, if the series

$$f(x) = \sum_{n=0}^{\infty} c_n \left(x - \frac{a+b}{2}\right)^n \tag{5.6.31}$$

converges for $\left|x - \frac{a+b}{2}\right| > (b-a)/2$.

(ii) The zeros $x_j^{(n)}$ and the corresponding weights $w_j^{(n)}$ are already tabulated for different values of n, or else they can be easily computed.

Example 7: An Oscillatory Integrand:

$$\int_0^{2\pi} x \sin(\ell x)\cos(x)dx\,.$$

Table 5.6.5: Results for Example 7??

ℓ	Exact	32-Point Legendre Quadrature
1	-1.57079	-1.57079
2	-4.18879	-4.18428
4	-1.67552	-1.67565
10	-.63467	-.63402
20	-.31495	-1.20925
30	-.20967	-1.58222

This integral was approximated by 32-point Gauss-Legendre quadrature. The results are given in Table 5.6.5.

Problems

5.6.1 Show that the sequence of polynomials $\{\psi_n\}_{n=0}^{\infty}$ constructed in (5.5.5) satisfies (5.5.3). Hint: Note first of all that $\{\psi_n\}_{n=0}^{N}$ is an independent set. For our inductive hypothesis assume that $\{\psi_n\}_{n=0}^{N-1}$ are orthonormal (they clearly satisfy $(\psi_n, \psi_n) = 1$ in (5.5.3)). Now compute $(\psi_N, \psi_j) = (\theta_N, \theta_N)^{-1/2}(\theta_N, \psi_j)$ for $j < N$ using (5.5.6) and independent of $\{\psi_n\}_{n=0}^{N}$.

5.6.2 Show that if $\pi_j(x)$ is an arbitrary polynomial of degree $j < n$ then $(\psi_n, \pi_j) = 0$.

5.6.3 Show that the sequence $\{\theta_n\}_{n=0}^{\infty}$ satisfies the recurrence relation

$$\begin{aligned} \theta_0 &\equiv 1 \qquad\qquad \theta_1(x) = x - \beta_1 \\ \theta_n(x) &= (x-\beta_n)\theta_{n-1}(x) - \gamma_{n-1}\theta_{n-2}(x)\ , \quad n \geq 2 \end{aligned}$$

where

$$\beta_n = \frac{(x\,\theta_{n-1}, \theta_{n-1})}{(\theta_{n-1}, \theta_{n-1})}\ ,\ \gamma_{n-1} = \frac{(x\,\theta_{n-1}, \theta_{n-2})}{(\theta_{n-2}, \theta_{n-2})}\ .$$

Hint: Using the notation in (5.6.3) write

$$\begin{aligned} \theta_n(x) - x\,\theta_{n-1}(x) &= -\beta_n\theta_{n-1}(x) - \gamma_{n-2}\theta_{n-2} + c_{n-3}\theta_{n-3} \\ &\quad + \cdots + c_1\theta_1(x) + c_0\theta_0(x) \end{aligned}$$

and use the orthogonality of $\{\theta_j\}_{j=0}^{n-3}$ to show that $c_j = 0$ for $j = 0, l \ldots, n-3$. Now use the orthogonality of θ_{n-1} and θ_n to find β_n and γ_{n-1}.

5.6.4 If $[a, b] = [-1, 1]$ and $w(x) = 1$ in (5.6.3) the resulting orthonormal polynomials are called the Legendre polynomials. Use Problem 5.6.3 to find the first five Legendre polynomials. Verify that the roots $x_j^{(n)}$ in Table 5.6.1 are correct $(n = 2, 3, 4, 5)$.

5.6.5 Verify Lemma 5.6.2.

5.6.6 How many evaluation points are required to evaluate $\int_{-1}^{1}(1-x^2)^{-1/2}e^x dx$ accurate to eight decimals using the Gauss-Chebyshev quadrature (5.6.26)?

5.6.7 Prove that the weights $w_j^{(n)}$ in (5.6.18) are given by

$$w_j^{(n)} = -\frac{k_{n+1}}{k_n \psi_{n+1}(x_j)\psi_n'(x_j)}$$

where k_n is defined in (5.6.4).

5.6.8 If $w(x) = (1 - x^2)^{1/2}$, $a = -1$, $b = +1$ and $f \in C^{2n}[-1, 1]$ then

$$\int_{-1}^{1} (1 - x^2)^{1/2} f(x) dx = \sum_{j=1}^{n} w_j^{(n)} f(x_j^{(n)}) + \frac{\pi}{2^{2n+1}(2n)!} f^{2n}(\xi)$$

for some $\zeta \in (-1, 1)$, where

$$x_j^{(n)} = \cos\left(\frac{j\pi}{n+1}\right), \; w_j^{(n)} = \pi \sin^2\left(\frac{j\pi}{n+1}\right).$$

This is the Gauss-Chebyshev quadrature based on the Chebyshev polynomials of the second kind $u_n(x) = \sin((n + 1)\theta)/\sin\theta$, $\cos\theta = x$.

5.6.9 Show that the quadrature

$$\int_1^3 f(x)dx = \frac{5}{9} f(2 - \sqrt{315}) + \frac{8}{9} f(2) + \frac{5}{9} f(2 + \sqrt{315})$$

is exact when f is a polynomial of degree 5.

5.6.10 Let $\{\psi_n\}$ be defined as in (5.6.5). Prove that

$$\sum_{j=1}^{n} \int_a^b w(x) \left[\frac{\psi_n(x)}{(x - x_j^{(n)})\psi_n'(x_j^{(n)})}\right]^2 dx = \sum_{j=1}^{n} w_j^{(n)} = \int_a^b w(x)dx .$$

5.6.11 Find x_j and w_j so that the formula

$$\int_0^1 x^{2/3} f(x)dx = \sum_{j=1}^{5} w_j f(x_j)$$

is exact when f is a polynomial of degree nine.

5.7 Quadratures Based on the Trapezoidal Rule

Let us briefly recall various features of the quadrature formulas constructed in the previous sections. The trapezoidal and mid-ordinate formulas are very simple to use on a computer. Using (5.3.11), it was possible to use previously computed evaluation points by halving the step-size h. A disadvantage of the trapezoidal and mid-ordinate rules is that they converge so slowly, even for smooth functions, that it is usually impossible to achieve more than five significant figures of accuracy using eight significant figure arithmetic. This situation is often remedied by using the Romberg algorithm; however, when singularities are present at endpoints of integration, the Romberg method, as well as the trapezoidal and mid-ordinate methods, usually fails.

Due to the relatively few points they require, the Gaussian formulas often yield very accurate results in the case when the integrand is smooth. Their disadvantage is that to increase the accuracy, we cannot use previously computed evaluation points, and it is thus inconvenient to obtain an estimate of the error on a posteriori basis. Furthermore, in the case when singularities are present at an endpoint of integration, i.e., when in the approximation

$$\int_a^b w(x)f(x)dx \simeq \sum_{j=1}^{n} w_j^{(n)} f(x_j^{(n)})$$

the function f also has singularities the Gaussian formulas are not much better than the mid-ordinate formulas.

Ideally, one would like formulas that are simple to apply on a computer, for which one can use previously computed evaluation points via a device such as that of (5.3.11), which converge as rapidly as the trapezoidal formula in Table 5.4.2, so that we can easily estimate the error a posteriori, and which are usually insensitive to singularities located at endpoints of integration. While there are no universal-type quadrature formulas that yield accurate results for all integrands (c.f. [5] and Problems 5.7.9–5.7.14), the formulas that we construct in this section do have the desirable features that we have just described. We only list three formulas; further generalizations and the effectiveness of the formulas when singularities are present at endpoints of integration can be found in the literature [6].

Theorem 5.7.1 *(a) Let $f^{(k)}(x)$ exist on the interval $(-\infty, \infty)$, and let*

$$\int_{-\infty}^{\infty} |f^{(k)}(x)|dx < \infty \tag{5.7.1}$$

for $k = 0, 1, 2, 3, \ldots$. Then for every $\alpha > 0$

$$\int_{-\infty}^{\infty} f(x)dx - h \sum_{k=-\infty}^{\infty} f(kh) = 0(h^{\alpha}) \tag{5.7.2}$$

as $h \to 0$.

(b) Let $F^{(k)}(x)$ exist on the interval $(0, \infty)$, and let

$$\int_{0}^{\infty} y^k |F^{(k)}(y)|dy < \infty \tag{5.7.3}$$

for $k = 0, 1, 2, 3, \ldots$. Then for every $\alpha > 0$

$$\int_{0}^{\infty} F(y)dy - h \sum_{k=-\infty}^{\infty} e^{kh} F(e^{kh}) = 0(h^{\alpha}) \tag{5.7.4}$$

as $h \to 0$.

(c) Let $\mathcal{F}^{(k)}(x)$ exist on the interval $(-1, 1)$, and let

$$\int_{-1}^{1} (1 - x^2)^k |\mathcal{F}^{(k)}(x)|dx < \infty \tag{5.7.5}$$

for $k = 0, 1, 2, 3, \ldots$. Then for every $\alpha > 0$

$$\int_{-1}^{1} \mathcal{F}(x)dx - h \sum_{k=-\infty}^{\infty} \frac{2e^{kh}}{(1 + e^{kh})^2} \mathcal{F}\left(\frac{e^{kh} - 1}{e^{kh} + 1}\right) = 0(h^{\alpha}) \tag{5.7.6}$$

as $h \to 0$.

Before proving this theorem, we state some properties of the formulas, and we describe an effective algorithm for using them. Each of the formulas takes the form

$$\int_a^b g(x)dx \cong h \sum_{k=-\infty}^{\infty} w_k(h) g(x_k(h)), \tag{5.7.7}$$

where, for example, in formula (5.7.6), $a = -1$, $b = 1$, $w_k(h) = 2e^{kh}/(1+e^{kh})^2$, and $x_k(h) = (e^{kh}-1)/(e^{kh}+1)$. For each of the formulas $w_{2k}(h/2) = w_k(h)$, $x_{2k}(h/2) = x_k(h)$. These remarks lead us to the following algorithm for evaluating $\int_a^b g(x)dx$ to within ϵ, where $\epsilon > 0$ is given.

Algorithm 5.7.2 Quadrature Based on the Trapezoidal Rule

Pick c and d, $a < c < d < b$, such that

$$\int_a^c |g(x)|dx < \frac{\epsilon}{3} \quad \text{and} \quad \int_d^b |g(x)|dx < \frac{\epsilon}{3}$$

Pick $h > 0$.

Evaluate $\quad T_h(g) \equiv h \sum_{x_k(h)\in(c,d)} w_k(h) g(x_k(h))$

Evaluate $\quad M_h(g) \equiv h \sum_{x_{2k-1}(h/2)\in(c,d)} w_{2k-1}(h/2) g(x_{2k-1}(h/2))$

Note $\quad T_{h/2}(h) = \frac{1}{2}\left[T_h(g) + M_h(g)\right]$

If $|T_{h/2}(g) - T_h(g)| < \epsilon/3$

then accept $T_{h/2}(g)$

else

$h \leftarrow h/2$

Return

Proof of Theorem 5.7.1

(a) This is a direct consequence of Corollary 5.4.7

(b) Here we set

$$x = e^t \tag{5.7.8}$$

in the integral in (5.6.4), and then apply the result (5.7.2), to get

$$\int_0^\infty F(x)dx = \int_{-\infty}^\infty e^t F(e^t) = h \sum_{k=-\infty}^\infty e^{kh} F(e^{kh}) = 0(h^\alpha) \tag{5.7.9}$$

as $h \to 0$, for all $\alpha > 0$, provided that

$$\int_{-\infty}^\infty |(e^t F(e^t))^{(k)}| dt < \infty \tag{5.7.10}$$

for $k = 0, 1, 2, 3, \ldots$. Now it is readily verified by induction (see Problem 5.7.4) that there are constants $a_{k\ell}$, $\ell = 0, 1, \ldots, k-1$, such that

$$(e^t F(e^t))^{(k)} = (e^{(k+1)t}) F^{(k)}(e^t) + \sum_{\ell=0}^{k-1} a_{k\ell} (e^{(\ell+1)t}) F^{(\ell)}(e^t) \tag{5.7.11}$$

where the sum on the right is zero if $k = 0$. Hence, if

$$\int_0^\infty y^k |F^{(k)}(y)| dy = \int_{-\infty}^\infty e^{(k+1)t} |F^{(k)}(e^t)| dt < \infty \tag{5.7.12}$$

for $k = 0, 1, 2, 3, \ldots$, then from (5.7.11) it follows that (5.7.10) is satisfied.

(c) For this case we set

$$x = \tanh \frac{1}{2} w \tag{5.7.13}$$

in the integral on the right of (5.7.6), and substitute into (5.6.2) to get

$$\begin{aligned} \int_{-1}^1 \mathcal{F}(x) dx &= \int_{-\infty}^\infty \frac{1}{2} \operatorname{sech}^2 \left(\frac{1}{2} w \right) \mathcal{F} \left(\tanh \frac{1}{2} w \right) dw \\ &= h \sum_{k=-\infty}^\infty \left(\frac{2e^{kh}}{(1+e^{kh})^2} \right) \mathcal{F} \left(\frac{e^{kh}-1}{e^{kh}+1} \right) + 0(h^\alpha) \end{aligned} \tag{5.7.14}$$

as $h \to 0$, for all $\alpha > 0$, if the function $f(w) = (1/2)\operatorname{sech}^2(w/2)\mathcal{F}(\tanh(w/2))$ satisfies (5.7.1) for $k = 0, 1, 2, \ldots$. Now we can verify by induction (see Problems 5.7.5, 5.7.6 and 5.7.7) that there are functions $b_{k\ell}(x)$,

$\ell = 0, 1, \ldots, k-1$, which are uniformly bounded for $-\infty \le x \le \infty$, such that

$$\begin{aligned}((1/2)\mathrm{sech}^2(x/2)\psi(\tanh x/2)) &= \frac{\mathrm{sech}^2 x/2}{2}\,\psi^{(k)}(\tanh(x/2)) \\ &\quad + \sum_{\ell=0}^{k-1} b_{k\ell}(x)\mathrm{sech}^{2\ell+2}(x/2)\psi^{(\ell)}(\tanh x/2)\quad .\end{aligned} \tag{5.7.15}$$

Hence if

$$\begin{aligned}\int_{-1}^{1} (1 &- x^2)^{(k)}\mathcal{F}^{(k)}(x)\,dx \\ &= \frac{1}{2}\int_{-\infty}^{\infty} |(\mathrm{sech}^2(x/2))^{(k+1)}|\;|\mathcal{F}^{(k)}(\tanh(x/2))|dx < \infty\end{aligned} \tag{5.7.16}$$

for $k = 0, 1, 2, \ldots$, then (5.7.5) is satisfied.

Example 5.7.3 We approximate

$$\int_4^\infty \frac{e^{-x^2}}{\sqrt{2\pi}}\,dx = .54508\ 23808\ 67 \times 10^{-8}$$

by use of (5.7.4). Here we first replace x by $4+y$, and then apply (5.2.4) in the Algorithm 5.7.2. The results are contained in Table 5.7.

Table 5.7.1:

h	Number of Points	Results $\times 10^8$
$\log 2$	23	.545080
$\frac{1}{2}\log 2$	79	.54508238081
$\frac{1}{4}\log 2$	149	.545082380867

Example 2: We have already seen the effectiveness of Gaussian quadrature (see Example 6 in Section 6) for evaluating an integral of the form

$$I = \int_{-1}^{1} e^x\,dx\,.$$

Table 5.7.2: Comparison of Number of Points

Trap Rule	Gauss	6.6	Accuracy
900	4	21	6.55 − 7
912,870	7	83	4.29 − 13
9×10^{11}	9	329	1.84 − 25

We evaluate this integral using the trapezoidal rule, the Gauss-Legendre rule, and the formula of (5.7.6), and we compare the number of points required to achieve the same accuracy. The results are contained in Table 5.7.

Thus the formula of (5.7.6) is not as accurate as Gaussian quadrature for some integrands, although in the case of this particular example, it is considerably more accurate than the trapezoidal rule.

We do not want to leave the reader with the impression that the formulas derived in this section are universal, since formulas that converge rapidly for all integrands do not exist (see Problems 5.7.9–5.7.14). For example, when evaluating

$$\int_{-\infty}^{\infty} (1+x^2)^{-1} dx$$

by (5.7.2) the error can be shown to be $4\pi e^{-2\pi/h}/(1-e^{-2\pi/h})$. Although the error converges to zero very rapidly as a function of h, many evaluation points are required, since the integrand converges to zero slowly as $x \to \pm\infty$. Note, however, that (5.5.4) works well for evaluating $\int_0^\infty (1+x^{-2})dx$. Although $\int_a^\infty [(\sin x)/x]dx$ exists for every finite a, we cannot evaluate this integral by use of the formula (5.7.4), since the resulting infinite sum is divergent for every $h > 0$. Finally, the formula of (5.7.6) fails to converge rapidly for the valuation of $\int_0^1 x\sin(1/x)dx$.

Problems

5.7.1 Let $\alpha \in (0,2)$. Find constants $c_1 > 0$ and $c_2 > 0$, such that

$$\frac{c_1}{n^\alpha} < \int_0^1 x^{\alpha-1}dx - \frac{1}{n}\sum_{k=1}^{n}\left(\frac{2k-1}{2n}\right)^{\alpha-1} < \frac{2}{n^\alpha}\,, \quad n = 1,2,3,\ldots.$$

5.7.2 Find $\int_{-1}^1 (1-x^2)^{-1/2}dx$ accurate to six significant figures using the formula (5.7.6) in the Algorithm 7.2.

5.7.3 Evaluate $\int_0^\infty y^{-1/2}(1+y)^{-1}dy$ correct to six significant figures, using (5.7.4) in Algorithm 5.2.

5.7.4 Verify (5.7.11) by showing that the constants $a_{k\ell}$ satisfy the recurrence relations

$$\begin{aligned} a_{k+1,\ell} &= (\ell+1)a_{k\ell} + a_{k,\ell-1}\ , \quad \ell = 0,1,\ldots,k-1 \\ a_{k+1,k} &= k+1+a_{k,k-1}\ . \end{aligned}$$

5.7.5 Verify that there are constants α_{jk} such that

$$(\tanh(x/2))^{(2k-1)} = \sum_{j=1}^{2k-1} \alpha_{jk}\text{sech}^{2j}(x/2)\ , \quad k = 1,2,3,\ldots.$$

5.7.6 Verify that these are constants β_{jk} such that

$$(\tanh(x/2))^{(2k)} = \tanh(x/2)\sum_{j=0}^{2k} \beta_{jk}\text{sech}^{2j}(x/2)\ , \quad k = 0,1,2,\ldots.$$

5.7.7 Use the results of Problems 5.7.5 and 5.7.6 to verify (5.7.15), where $b_{k\ell}^{(j)}(x)$ is uniformly bounded for $-\infty \le x \le \infty$.

5.7.8 Show that if $\int_{-\infty}^\infty |f^{(k)}(x)|dx < \infty$ for $h = 0,1,2,\ldots$, then $f^{(k)}(x) \to 0$ as $x \to \pm\infty$.

5.7.9 Let $Q_n(f)$ be defined by

$$Q_n(f) = \frac{1}{2^{n-1}}\left[f\left(\frac{1}{2^n}\right) + f\left(\frac{3}{2^n}\right) + \cdots + f\left(\frac{2^n-1}{2^n}\right)\right].$$

Prove that $Q_n(f) \to \int_0^1 f(x)dx$ as $n \to \infty$ for all $f \in C[0,1]$.

5.7.10 Let π_n denote the set of points $\left\{\frac{2k-1}{2^n}\right\}_{k=1}^{2^{n-1}}$, $n = 1,2,\ldots$ and let $s_n(x)$ denote the linear spline that is 1 for $x \in \pi_n$, and zero for all points halfway between two consecutive points of π_n as well as for $x = 0$ and $x = 1$. Prove that if $\sum_{n=1}^\infty |\alpha_n| < \infty$, then the function f defined by $f(x) = \sum_{n=1}^\infty \alpha_n s_n(x)$ is in $C[0,1]$.

5.7.11 In the notation of Problems 5.7.9 and 5.7.10, prove that $\int_0^1 s_n(x)dx = 1/2$, $n = 1, 2, 3, \ldots$, and also that $Q_i(s_j) = 1/2$ if $j < i$, 1 if $j = i$, and 0 if $j > i$.

5.7.12 Let $a_n > 0$ for $n = 1, 2, \ldots$ and $a_1 > a_2 > \cdots$ with $a_n \to 0$ as $n \to \infty$. Let $\alpha_1 = 0$ and α_n $(n \geq 2)$ be defined by $\alpha_{n+1} = (1/2)\alpha_n + a_n - a_{n+1}$, $n = 1, 2, \ldots$. Prove that if f is defined as in ???6.10 then the function $f = \sum_{n=1}^{\infty} \alpha_n s_n(x) \in C[0, 1]$.

5.7.13 Prove that if f is defined as in Problem **??**, and Q_n as in Problem 5.6.9, then

$$\int_0^1 f(x)dx - Q_n(f) = a_n \ , \quad n = 1, 2, 3 \ldots .$$

5.7.14 Prove that the function f defined in Problem **??** satisfies $\|f(x)\| \leq 2a_1$, $0 \leq x \leq 1$.