Chapter 8

Integration Using Chebyshev Polynomials

In this chapter we show how Chebyshev polynomials and some of their fundamental properties can be made to play an important part in two key techniques of numerical integration.

- Gaussian quadrature estimates an integral by combining values of the integrand at zeros of orthogonal polynomials. We consider the special case of *Gauss–Chebyshev quadrature*, where particularly simple procedures follow for suitably weighted integrands.
- One can approximately integrate a function by expanding it in a series and then integrating a partial sum of the series. We show that, for Chebyshev expansions, this process — essentially the *Clenshaw–Curtis method* — is readily analysed and again provides a natural procedure for appropriately weighted integrands.

Although this could be viewed as an 'applications' chapter, which in an introductory sense it certainly is, our aim here is primarily to derive further basic properties of Chebyshev polynomials.

8.1 Indefinite integration with Chebyshev series

If we wish to approximate the indefinite integral

$$h(X) = \int_{-1}^{X} w(x)f(x)\,\mathrm{d}x,$$

where $-1 < X \leq 1$, it may be possible to do so by approximating $f(x)$ on $[-1, 1]$ by an nth degree polynomial $f_n(x)$ and integrating $w(x)f_n(x)$ between -1 and X, giving the approximation

$$h(X) \simeq h_n(X) = \int_{-1}^{X} w(x)f_n(x)\,\mathrm{d}x. \tag{8.1}$$

Suppose, in particular, that the weight $w(x)$ is one of the four functions

$$w(x) = \frac{1}{\sqrt{1-x^2}},\ 1,\ \frac{1}{\sqrt{1-x}},\ \frac{1}{\sqrt{1+x}}, \tag{8.2}$$

and that we take $f_n(x)$ as the partial sum of the expansion of $f(x)$ in Chebyshev polynomials of the corresponding one of the four kinds

$$P_k(x) = T_k(x),\ U_k(x),\ V_k(x),\ W_k(x). \tag{8.3}$$

Then we can use the fact that (excluding the case where $P_k(x) = T_k(x)$ with $k = 0$)

$$\int_{-1}^{X} w(x)P_k(x)\,\mathrm{d}x = C_k(X)Q_k(X) - C_k(-1)Q_k(-1)$$

where

$$Q_k(X) = U_{k-1}(X),\ T_{k+1}(X),\ W_k(X),\ V_k(X) \tag{8.4a}$$

and

$$C_k(X) = -\frac{\sqrt{1-X^2}}{k},\ \frac{1}{k+1},\ 2\frac{\sqrt{1-X}}{k+\frac{1}{2}},\ -2\frac{\sqrt{1+X}}{k+\frac{1}{2}}, \tag{8.4b}$$

respectively. (Note that $C_k(-1) = 0$ in the first and fourth cases.) This follows immediately from the fact that if $x = \cos\theta$ then we have

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}x}\sin k\theta &= -\frac{k\cos k\theta}{\sin\theta},\\
\frac{\mathrm{d}}{\mathrm{d}x}\cos(k+1)\theta &= \frac{(k+1)\sin(k+1)\theta}{\sin\theta},\\
\frac{\mathrm{d}}{\mathrm{d}x}\sin(k+\tfrac{1}{2})\theta &= -\frac{(k+\frac{1}{2})\cos(k+\frac{1}{2})\theta}{\sin\theta},\\
\frac{\mathrm{d}}{\mathrm{d}x}\cos(k+\tfrac{1}{2})\theta &= \frac{(k+\frac{1}{2})\sin(k+\frac{1}{2})\theta}{\sin\theta}.
\end{aligned}$$

In the excluded case, we use

$$\frac{\mathrm{d}}{\mathrm{d}x}\theta = -\frac{1}{\sin\theta}$$

to give

$$\int_{-1}^{X} \frac{1}{\sqrt{1-x^2}} T_0(x)\,\mathrm{d}x = \arccos(-1) - \arccos X = \pi - \arccos X.$$

Thus, for each of the weight functions (8.2) we are able to integrate the weighted polynomial and obtain the approximation $h_n(X)$ explicitly. Suppose that

$$f_n(x) = {\sum_{k=0}^{n}}' a_k T_k(x)\ [P_k = T_k] \quad\text{or}\quad \sum_{k=0}^{n} a_k P_k(x)\ [P_k = U_k,\, V_k,\, W_k]. \tag{8.5}$$

Then in the first case

$$\begin{aligned}
h_n(X) &= {\sum_{k=0}^{n}}' a_k \int_{-1}^{X} w(x)T_k(x)\,\mathrm{d}x = \\
&= \tfrac{1}{2}a_0(\pi - \arccos X) - \sum_{k=1}^{n} a_k \frac{\sqrt{1-X^2}}{k} U_{k-1}(X),
\end{aligned} \tag{8.6}$$

while in the second, third and fourth cases

$$h_n(X) = \sum_{k=0}^{n} a_k \int_{-1}^{X} w(x) P_k(x)\,\mathrm{d}x = \sum_{k=0}^{n} a_k \left[C_k(x) Q_k(x) \right]_{-1}^{X}. \tag{8.7}$$

The above procedure is a very reliable one, as the following theorem demonstrates.

Theorem 8.1 *If $f(x)$ is $\mathcal{L}_2$-integrable with respect to one of the weights $w(x)$, as defined by (8.2), and $h_n(X)$ is defined by (8.6) or (8.7) as appropriate, if $Q_k(X)$ and $C_k(X)$ are defined by (8.4), and if a_k are the* exact *coefficients of the expansion of $f(x)$ in Chebyshev polynomials of the corresponding kind, then $h_n(X)$ converges uniformly to $h(X)$ on $[-1, 1]$.*

Proof: The idea of the proof is the same in all four cases. We give details of the second case here, and leave the others as exercises (Problems 1 and 2).

For $P_k = U_k$, $w = 1$,

$$\begin{aligned} h_n(X) &= \int_{-1}^{X} f_n(x)\,\mathrm{d}x \\ &= \int_{-1}^{X} \sum_{k=0}^{n} a_k \sin(k+1)\theta\,\mathrm{d}\theta. \end{aligned}$$

Thus the integrand is the partial Fourier sine series expansion of $\sin\theta\, f(\cos\theta)$, which converges in $\mathcal{L}_2$ and hence in $\mathcal{L}_1$ (Theorems 5.2 and 5.5).

Now

$$\begin{aligned} \|h - h_n\|_\infty &= \max_X \left| \int_{-1}^{X} \{f(x) - f_n(x)\}\,\mathrm{d}x \right| \\ &\le \max_X \int_{-1}^{X} |f(x) - f_n(x)|\,\mathrm{d}x \\ &= \int_{-1}^{1} |f(x) - f_n(x)|\,\mathrm{d}x \\ &= \int_{0}^{\pi} \left| \sin\theta\, f(\cos\theta) - \sum_{k=0}^{n} a_k \sin(k+1)\theta \right| \mathrm{d}\theta \\ &\to 0, \quad n \to \infty. \end{aligned}$$

Hence h_n converges uniformly to h. ●●

The coefficients a_k in (8.5) have been assumed to be exactly equal to the relevant Chebyshev series coefficients. In practice, we most often approximate these by the corresponding coefficients in a Chebyshev interpolation polynomial (see Chapter 6) — effectively evaluating the integral that defines a_k by the trapezoidal rule (see Section 6.2). In some circumstances, we may need to calculate the Chebyshev coefficients more accurately than this.

The method followed above is equivalent to methods well known in the literature. For the first choice ($P_k = T_k$) the method is that of Clenshaw & Curtis (1960) and for the second choice ($P_k = U_k$) that of Filippi (1964).

The analysis of Section 8.1 is taken mainly from Mason & Elliott (1995, and related papers).

8.2 Gauss–Chebyshev quadrature

Suppose that we now wish to calculate a definite integral of $f(x)$ with weight $w(x)$, namely

$$I = \int_a^b f(x)w(x)\,\mathrm{d}x. \tag{8.8}$$

Suppose also that I is to be approximated in the form

$$I \simeq \sum_{k=1}^{n} A_k f(x_k) \tag{8.9}$$

where A_k are certain coefficients and $\{x_k\}$ are certain abscissae in $[a, b]$ (all to be determined). The idea of Gauss quadrature is to find that formula (8.9) that gives an exact result for all polynomials of as high a degree as possible.

If $J_{n-1}f(x)$ is the polynomial of degree $n-1$ which interpolates $f(x)$ in any n distinct points $x_1, \ldots, x_n$, then

$$J_{n-1}f(x) = \sum_{k=1}^{n} f(x_k)\ell_k(x) \tag{8.10}$$

where ℓ_k is the Lagrange polynomial (as in (6.5))

$$\ell_k(x) = \prod_{\substack{r=1\\ r\neq k}}^{n} \left(\frac{x - x_r}{x_k - x_r}\right) \tag{8.11}$$

The polynomial $J_{n-1}f(x)$ has the integral

$$\begin{aligned} I_n &= \int_a^b J_{n-1}f(x)w(x)\,\mathrm{d}x \\ &= \sum_{k=1}^{n} f(x_k) \int_a^b w(x)\ell_k(x)\,\mathrm{d}x \\ &= \sum_{k=1}^{n} A_k f(x_k) \end{aligned}$$

provided that the coefficients A_k are chosen to be

$$A_k = \int_a^b w(x)\ell_k(x)\,\mathrm{d}x. \tag{8.12}$$

With any n distinct abscissae, therefore, and with this choice (8.12) of coefficients, the formula (8.9) certainly gives an exact result whenever $f(x)$ is a polynomial of degree $n-1$ or less. We can improve on this degree, however, by a suitable choice of abscissae.

Notice too that, for general abscissae, there is no control over the signs and magnitudes of the coefficients A_k, so that evaluation of the formula (8.9) may involve heavy cancellation between large terms of opposite signs, and consequent large rounding error. When we choose the abscissae to maximise the degree of exactness, however, it can be shown that this problem ceases to arise.

Theorem 8.2 *If x_k ($k = 1,\ldots,n$) are the n zeros of $\phi_n(x)$, and $\{\phi_k : k = 0,1,2,\ldots\}$ is the system of polynomials, ϕ_k having the exact degree k, orthogonal with respect to $w(x)$ on $[a,b]$, then (8.9) with coefficients (8.12) gives an exact result whenever $f(x)$ is a polynomial of degree $2n-1$ or less. Moreover, all the coefficients A_k are positive in this case.*

Proof: Since $\phi_n(x)$ is a polynomial exactly of degree n, any polynomial $f(x)$ of degree $2n-1$ can be written (using long division by ϕ_n) in the form

$$f(x) = \phi_n(x)Q(x) + J_{n-1}f(x)$$

where $Q(x)$ and $J_{n-1}f(x)$ are polynomials each of degree at most $n-1$. Then

$$\int_a^b f(x)w(x)\,\mathrm{d}x = \int_a^b \phi_n(x)Q(x)w(x)\,\mathrm{d}x + \int_a^b J_{n-1}f(x)w(x)\,\mathrm{d}x. \tag{8.13}$$

Now $\phi_n(x)$ is orthogonal to all polynomials of degree less than n, so that the first integral on the right-hand side of (8.13) vanishes. Thus

$$\begin{aligned}\int_a^b f(x)w(x)\,\mathrm{d}x &= \int_a^b J_{n-1}f(x)w(x)\,\mathrm{d}x \\ &= \sum_{k=1}^n A_k J_{n-1}f(x_k)\end{aligned}$$

since the coefficients have been chosen to give an exact result for polynomials of degree less than n. But now

$$f(x_k) = \phi_n(x_k)Q(x_k) + J_{n-1}f(x_k) = J_{n-1}f(x_k),$$

since x_k is a zero of $\phi_n(x)$. Hence

$$\int_a^b f(x)w(x)\,\mathrm{d}x = \sum_{k=1}^n A_k f(x_k),$$

and so (8.9) gives an exact result for $f(x)$, as required.

To show that the coefficients A_k are positive, we need only notice that $\ell_k(x)^2$ is a polynomial of degree $2n-2$, and is therefore integrated exactly, so that

$$A_k \equiv \sum_{j=1}^{n} A_j \ell_k(x_j)^2 = \int_a^b \ell_k(x)^2 w(x)\,\mathrm{d}x > 0$$

for each k. ●●

Thus we can expect to obtain very accurate integrals with the formula (8.9), and the formula should be numerically stable.

When the interval $[a,b]$ is $[-1,1]$ and the orthogonal polynomials $\phi_n(x)$ are one of the four kinds of Chebyshev polynomials, then the weight function $w(x)$ is $(1-x^2)^{-\frac{1}{2}}$, $(1-x^2)^{\frac{1}{2}}$, $(1+x)^{\frac{1}{2}}(1-x)^{-\frac{1}{2}}$ or $(1-x)^{\frac{1}{2}}(1+x)^{-\frac{1}{2}}$ and the zeros x_k are known explicitly. It remains to determine the coefficients A_k, which we may do by making use of the following lemma.

Lemma 8.3

$$\begin{aligned} ⨍_0^\pi \frac{\cos n\theta}{\cos\theta - \cos\phi}\,\mathrm{d}\theta &= \pi \frac{\sin n\phi}{\sin\phi}, \\ ⨍_0^\pi \frac{\sin n\theta\ \sin\theta}{\cos\theta - \cos\phi}\,\mathrm{d}\theta &= -\pi\cos n\phi, \end{aligned}$$

for any ϕ *in* $[0,\pi]$, $n = 1, 2, 3, \ldots$.

(We have stated this lemma in terms of the 'Cauchy principal value' integral $⨍ \cdots \mathrm{d}\theta$ since, if we allow ϕ to take an arbitrary value, the integrands have a non-integrable singularity at $\theta = \phi$. However, when we come to apply the lemma in this chapter, $\theta = \phi$ will always turn out to be a zero of the numerator, so that the singularity will in fact be removable and the principal value integrals will be equivalent to integrals in the ordinary sense.)

Proof: The lemma can be proved by induction on n, provided that we first establish the $n = 0$ case of the first result

$$⨍_0^\pi \frac{1}{\cos\theta - \cos\phi}\,\mathrm{d}\theta = 0.$$

We may do this as follows. Since $\cos\theta$ is an even function, we have

$$\begin{aligned} &⨍_0^\pi \frac{1}{\cos\theta - \cos\phi}\,\mathrm{d}\theta = \\ &= \tfrac{1}{2} ⨍_{-\pi}^\pi \frac{1}{\cos\theta - \cos\phi}\,\mathrm{d}\theta \\ &= ⨍_{-\pi}^\pi \frac{\mathrm{e}^{\mathrm{i}\theta}\,\mathrm{d}\theta}{(\mathrm{e}^{\mathrm{i}\theta} - \mathrm{e}^{\mathrm{i}\phi})(\mathrm{e}^{\mathrm{i}\theta} - \mathrm{e}^{-\mathrm{i}\phi})} \end{aligned}$$

$$= \oint_{|z|=1} \frac{-\mathrm{i}\,\mathrm{d}z}{(z - \mathrm{e}^{\mathrm{i}\phi})(z - \mathrm{e}^{-\mathrm{i}\phi})}$$

$$= \frac{-\mathrm{i}}{\mathrm{e}^{\mathrm{i}\phi} - \mathrm{e}^{-\mathrm{i}\phi}} \left[\oint_{|z|=1} \frac{\mathrm{d}z}{z - \mathrm{e}^{\mathrm{i}\phi}} - \oint_{|z|=1} \frac{\mathrm{d}z}{z - \mathrm{e}^{-\mathrm{i}\phi}} \right]$$

$$= \frac{-1}{2\sin\phi} [\mathrm{i}\pi - \mathrm{i}\pi] = 0.$$

We leave the subsequent induction as an exercise (Problem 3). ●●

The evaluation of A_k can now be carried out.

Theorem 8.4 *In the Gauss–Chebyshev formula*

$$\int_{-1}^{1} f(x)w(x)\,\mathrm{d}x \simeq \sum_{k=1}^{n} A_k f(x_k), \tag{8.14}$$

where $\{x_k\}$ *are the* n *zeros of* $\phi_n(x)$, *the coefficients* A_k *are as follows:*

1. *For* $w(x) = (1 - x^2)^{-\frac{1}{2}}$, $\phi_n(x) = T_n(x)$:

$$A_k = \frac{\pi}{n}.$$

2. *For* $w(x) = (1 - x^2)^{\frac{1}{2}}$, $\phi_n(x) = U_n(x)$:

$$A_k = \frac{\pi}{n+1}(1 - x_k^2).$$

3. *For* $w(x) = (1 - x)^{-\frac{1}{2}}(1 + x)^{\frac{1}{2}}$, $\phi_n(x) = V_n(x)$:

$$A_k = \frac{\pi}{n + \frac{1}{2}}(1 + x_k).$$

4. *For* $w(x) = (1 - x)^{\frac{1}{2}}(1 + x)^{-\frac{1}{2}}$, $\phi_n(x) = W_n(x)$:

$$A_k = \frac{\pi}{n + \frac{1}{2}}(1 - x_k).$$

Proof: We prove case 1 and leave case 2 as an exercise (Problem 4). We shall prove cases 3 and 4 a little later.

In case 1, writing

$$x_k = \cos\theta_k = \cos\frac{(k - \frac{1}{2})\pi}{n}$$

for the zeros of $T_n(x)$,

$$\begin{aligned} A_k &= \int_{-1}^{1} \frac{T_n(x)}{(x-x_k)\, n\, U_{n-1}(x_k)} \frac{\mathrm{d}x}{\sqrt{1-x^2}} \\ &= \int_0^{\pi} \frac{\cos n\theta \ \sin\theta_k}{(\cos\theta - \cos\theta_k)\, n\ \sin n\theta_k} \,\mathrm{d}\theta \\ &= \frac{\pi}{n}, \end{aligned}$$

using Corollary 6.4A and Lemma 8.3. ●●

Case 1 above is particularly convenient to use, since all weights are equal and the formula (8.9) can thus be evaluated with just $n-1$ additions and one multiplication.

EXAMPLE 8.1: To illustrate the exactness of (8.9) for polynomials of degree $\leq 2n-1$, consider $n=4$ and $f(x)=x^2$. Then

$$T_4(x) = 8x^4 - 8x^2 + 1$$

has zeros $x_1, \ldots, x_4$ with

$$x_1^2 = x_4^2 = \frac{2+\sqrt{2}}{4}, \quad x_2^2 = x_3^2 = \frac{2-\sqrt{2}}{4}.$$

Hence

$$\int_{-1}^{1} \frac{x^2}{\sqrt{1-x^2}}\,\mathrm{d}x \simeq \frac{\pi}{4}\sum_k x_k^2 = \frac{\pi}{4}\,2\left(\frac{2+\sqrt{2}}{4} + \frac{2-\sqrt{2}}{4}\right) = \frac{\pi}{2}$$

which is the exact value of the integral, as we expect. (See Problem 6 for a more challenging example.)

Cases 3 and 4 of Theorem 8.4, namely the Chebyshev polynomials of the third and fourth kinds, require a little more care. We first establish a lemma corresponding to Lemma 8.3.

Lemma 8.5

1.

$$\int_0^{\pi} \frac{\cos(n+\frac{1}{2})\theta}{\cos\theta - \cos\phi} \cos\tfrac{1}{2}\theta \,\mathrm{d}\theta = \frac{\pi}{2}\frac{\sin(n+\frac{1}{2})\phi}{\sin\frac{1}{2}\phi}.$$

2.

$$\int_0^{\pi} \frac{\sin(n+\frac{1}{2})\theta}{\cos\theta - \cos\phi} \sin\tfrac{1}{2}\theta \,\mathrm{d}\theta = -\frac{\pi}{2}\frac{\cos(n+\frac{1}{2})\phi}{\sin\frac{1}{2}\phi}.$$

Proof: (of the Lemma) From the first equation of Lemma 8.3, if we replace $\cos\theta$ by x and $\cos\phi$ by y,

$$\fint_{-1}^{1} \frac{T_n(x)}{x-y} \frac{\mathrm{d}x}{\sqrt{1-x^2}} = \pi U_{n-1}(y). \tag{8.15}$$

Writing $x = 2u^2 - 1$, $y = 2v^2 - 1$, where $u = \cos\frac{1}{2}\theta$, $v = \cos\frac{1}{2}\phi$,

$$\begin{aligned}
\fint_{-1}^{1} \left(\frac{1+x}{1-x}\right)^{\frac{1}{2}} \frac{V_n(x)}{x-y}\,\mathrm{d}x &= \fint_{0}^{1} \frac{2u}{\sqrt{1-u^2}} \frac{T_{2n+1}(u)}{u^2-v^2}\,\mathrm{d}u \\
&= \tfrac{1}{2} \fint_{-1}^{1} T_{2n+1}(u) \left(\frac{1}{u+v} + \frac{1}{u-v}\right) \frac{\mathrm{d}u}{\sqrt{1-u^2}} \\
&= \fint_{-1}^{1} \frac{T_{2n+1}(u)}{u-v} \frac{\mathrm{d}u}{\sqrt{1-u^2}} \\
&= \pi U_{2n}(v), \qquad \text{by (8.15)}.
\end{aligned}$$

Rewriting this in terms of θ and ϕ, we get

$$\fint_{0}^{\pi} \frac{1}{\sin\frac{1}{2}\theta} \frac{\cos(n+\frac{1}{2})\theta}{\cos\theta - \cos\phi} \sin\theta\,\mathrm{d}\theta = \pi \frac{\sin(2n+1)\frac{1}{2}\phi}{\sin\frac{1}{2}\phi}, \tag{8.16}$$

and this proves part 1 of the Lemma.

Part 2 may be proved similarly, starting from the second equation of Lemma 8.3, which gives

$$\fint_{-1}^{1} (1-x^2)^{\frac{1}{2}} \frac{U_{n-1}(x)}{x-y}\,\mathrm{d}x = \pi T_n(y),$$

and making similar substitutions. ●●

Proof: (of Theorem 8.4, case 3) Here

$$\begin{aligned}
A_k &= \fint_{-1}^{1} \left(\frac{1+x}{1-x}\right)^{\frac{1}{2}} \prod_{r\neq k} \left(\frac{x-x_r}{x_k-x_r}\right) \mathrm{d}x \\
&= \fint_{-1}^{1} \left(\frac{1+x}{1-x}\right)^{\frac{1}{2}} \frac{V_n(x)}{(x-x_k)V_n'(x_k)} \\
&= \fint_{0}^{\pi} \frac{1}{\sin\frac{1}{2}\theta} \frac{\cos(n+\frac{1}{2})\theta\ \cos\frac{1}{2}\theta_k\ \sin\theta_k\ \sin\theta}{(\cos\theta - \cos\theta_k)\ (n+\frac{1}{2})\ \sin(n+\frac{1}{2})\theta_k}\,\mathrm{d}\theta \\
&= \frac{2\pi}{n+\frac{1}{2}} \cos^2\tfrac{1}{2}\theta_k, \qquad \text{by (8.16)} \\
&= \frac{\pi}{n+\frac{1}{2}} (1+x_k).
\end{aligned}$$

Thus case 3 is proved. Case 4 follows, on replacing x by $-x$. ●●

EXAMPLE 8.2: To illustrate this case, consider, for example, $f(x) = x^2$ and $n = 2$ for case 3, so that

$$I = \int_{-1}^{1} \left(\frac{1+x}{1-x}\right)^{\frac{1}{2}} x^2 \, \mathrm{d}x.$$

Now $V_2(x) = 4x^2 - 2x - 1$ has zeros $x_1, x_2 = \frac{1}{4}(1 \pm \sqrt{5})$, with $x_1^2, x_2^2 = \frac{1}{8}(3 \pm \sqrt{5})$. Hence

$$\begin{aligned} I &\simeq \frac{2\pi}{5}[(1+x_1)x_1^2 + (1+x_2)x_2^2] \\ &= \frac{2\pi}{5}[\tfrac{1}{4}(5+\sqrt{5})\tfrac{1}{8}(3+\sqrt{5}) + \tfrac{1}{4}(5-\sqrt{5})\tfrac{1}{8}(3-\sqrt{5})] \\ &= \tfrac{1}{2}\pi. \end{aligned}$$

This is exact, as we can verify:

$$I = \int_0^{\pi} \frac{\cos\frac{1}{2}\theta}{\sin\frac{1}{2}\theta} (\cos\theta)^2 \sin\theta \, \mathrm{d}\theta = \int_0^{\pi} \tfrac{1}{2}(1+\cos\theta)(1+\cos 2\theta) \, \mathrm{d}\theta = \tfrac{1}{2}\pi.$$

The Gauss–Chebyshev quadrature formulae are the only Gauss formulae whose nodes x_k and weights A_k (given by Theorem 8.4) can be written down explicitly.

8.3 Quadrature methods of Clenshaw–Curtis type

8.3.1 Introduction

The Gauss–Chebyshev quadrature method of Section 8.2 is based on the continuous orthogonality properties of the Chebyshev polynomials. However, as we showed in Section 4.6, the four kinds of polynomials also have discrete orthogonality properties, and it is this kind of property that was exploited in the original quadrature method of Clenshaw & Curtis (1960). Their method has been developed in a considerable literature of papers by many authors (Piessens & Branders 1983, Adam 1987, Adam & Nobile 1991); a particularly nice presentation is given by Sloan & Smith (1978), who provide a version based on a general weight function together with a calculation of error estimates. Our treatment here is based on Sloan and Smith's formulation and techniques, which we can extend to all four kinds of Chebyshev polynomials.

The basic idea is to replace the integrand by an interpolating polynomial, and then to integrate this between the required limits. Suppose that we wish to determine the integral

$$I(f) := \int_{-1}^{1} w(x) f(x) \, \mathrm{d}x; \tag{8.17}$$

then we replace $f(x)$ by the polynomial $J_n f(x)$ of degree n which interpolates f in abscissae $\{x_k : k = 1, \ldots, n+1\}$, and hence we obtain the approximation

$$I_n(f) := \int_{-1}^{1} w(x) J_n f(x)\,\mathrm{d}x \tag{8.18}$$

to evaluate, either exactly or approximately. So far, this only repeats what we have said earlier. However, if Chebyshev polynomial abscissae are adopted as interpolation points then, as we saw in Section 6.3, discrete orthogonality properties lead to very economical interpolation formulae, expressing the polynomial $J_n f(x)$ in forms which can readily be integrated — in many cases exactly.

There are a few important cases in which Gauss–Chebyshev and Clenshaw–Curtis quadrature lead to the same formulae, although they differ in general.

8.3.2 First-kind formulae

Suppose that

$$J_n f(x) = \sum_{j=0}^{n} b_j T_j(x) \tag{8.19}$$

interpolates $f(x)$ in the zeros $\{x_k\}$ of $T_{n+1}(x)$. Then, using the discrete orthogonality results (4.40) and (4.42), we have

$$d_{ij} := \sum_{k=1}^{n+1} T_i(x_k) T_j(x_k) = 0, \quad i \neq j, \quad i, j \leq n \tag{8.20a}$$

and

$$d_{ii} = \begin{cases} (n+1), & i = 0, \\ \frac{1}{2}(n+1), & i \neq 0. \end{cases} \tag{8.20b}$$

Hence

$$\sum_{k=1}^{n+1} f(x_k) T_i(x_k) = \sum_{k=1}^{n+1} J_n f(x_k) T_i(x_k) = \sum_{j=0}^{n} b_j \sum_{k=1}^{n+1} T_i(x_k) T_j(x_k) = b_i d_{ii}$$

and so

$$b_i = \frac{1}{d_{ii}} \sum_{k=1}^{n+1} f(x_k) T_i(x_k). \tag{8.21}$$

From (8.18)

$$I_n(f) = \sum_{j=0}^{n} b_j a_j, \tag{8.22}$$

where

$$a_j = \int_{-1}^{1} w(x)T_j(x)\,\mathrm{d}x = \int_0^{\pi} w(\cos\theta)\ \cos j\theta\ \sin\theta\,\mathrm{d}\theta. \tag{8.23}$$

Formulae (8.21)–(8.23) give the quadrature rule

$$I_n(f) = \sum_{k=1}^{n+1} w_k f(x_k), \tag{8.24a}$$

$$w_k = \sum_{j=0}^{n} \frac{a_j}{d_{jj}} T_j(x_k) = \sum_{j=0}^{n}{}' \frac{2a_j}{n+1} T_j(x_k). \tag{8.24b}$$

Hence I_n is readily determined, provided that the integrals (8.23) defining a_j are straightforward to calculate.

- For the specific weighting

$$w(x) = (1-x^2)^{-\frac{1}{2}} \tag{8.25}$$

  we have

$$a_j = \int_{-1}^{1} (1-x^2)^{-\frac{1}{2}} T_j(x)\,\mathrm{d}x = \int_0^{\pi} \cos j\theta\,\mathrm{d}\theta = \begin{cases} \pi, & j=0, \\ 0, & j>0, \end{cases} \tag{8.26}$$

  giving

$$w_k = \frac{a_0}{d_{00}} T_0(x_k) = \frac{\pi}{n+1}.$$

  Hence

$$\int_{-1}^{1} f(x) \frac{\mathrm{d}x}{\sqrt{1-x^2}} \simeq I_n(f) = \frac{\pi}{n+1} \sum_{k=1}^{n+1} f(x_k). \tag{8.27}$$

  Thus we get the first-kind Gauss–Chebyshev formula of Theorem 8.4.

An alternative Clenshaw–Curtis formula may be obtained by defining $J_n f(x)$ to be the polynomial interpolating the values of $f(x)$ at the abscissae

$$y_k = \cos\frac{k\pi}{n}, \quad k = 0, \ldots, n,$$

which are the zeros of $(1-x^2)U_{n-1}(x)$. In this case we use the discrete orthogonality results (4.45) and (4.46) to give us

$$d_{ij} := \sum_{k=0}^{n}{}'' T_i(y_k)T_j(y_k) = 0, \quad i \neq j \tag{8.28a}$$

and

$$d_{ii} = \begin{cases} n, & i=0, i=n, \\ \frac{1}{2}n, & 0<i<n. \end{cases} \tag{8.28b}$$

We readily deduce, in place of (8.19), that

$$J_n f(x) = \sum_{j=0}^{n} b_j T_j(x) \tag{8.29}$$

where in this case

$$b_i = \frac{1}{d_{ii}} \sum_{k=0}^{n}{}'' f(y_k) T_i(y_k), \tag{8.30}$$

and that

$$I_n(f) = \sum_{j=0}^{n} b_j a_j$$

where a_j are given by the same formula (8.23) as before. This gives us the rule

$$I_n(f) = \sum_{k=0}^{n} w_k f(y_k) \tag{8.31a}$$

$$w_k = \sum_{j=0}^{n} \frac{a_j}{d_{jj}} T_j(y_k) = \sum_{j=0}^{n}{}'' \frac{2a_j}{n} T_j(y_k). \tag{8.31b}$$

- For $w(x) = (1-x^2)^{-\frac{1}{2}}$, this reduces to the formula

$$\int_{-1}^{1} f(x) \frac{dx}{\sqrt{1-x^2}} \simeq I_n(f) = \pi b_0 = \frac{\pi}{n} \sum_{j=0}^{n}{}'' f(y_k). \tag{8.32}$$

  This is nearly equivalent to the second-kind Gauss–Chebyshev formula of Theorem 8.4, applied to the function $\dfrac{f(x)}{1-x^2}$, except that account is taken of the values of $f(x)$ at the end points $x = \pm 1$. This may better reflect the inverse-square-root singularities of the integrand at these points.

8.3.3 Second-kind formulae

It is clear that the key to the development of a Clenshaw–Curtis integration method is the finding of a discrete orthogonality formula. In fact, there exist at least sixteen such formulae, listed in Problem 14 of Chapter 4, some of which are covered in Section 4.6.

An example of a second-kind discrete orthogonality formula, given by (4.50) and (4.51), is

$$d_{ij} = \sum_{k=1}^{n+1} (1-y_k^2) U_i(y_k) U_j(y_k) = \begin{cases} \frac{1}{2}(n+2), & i = j \le n, \\ 0, & i \ne j, \end{cases} \tag{8.33}$$

where $\{y_k\}$ are the zeros of $U_{n+1}(x)$:

$$y_k = \cos\frac{k\pi}{n+2}, \quad k = 1, \ldots, n+1.$$

To make use of this, we again approximate the required integral $I(f)$ of (8.17) by the integral $I_n(f)$ of the form (8.18), but now interpolating $f(x)$ by a function of the form

$$J_n f(x) = (1-x^2)^{\frac{1}{2}} \sum_{j=0}^{n} b_j U_j(x); \tag{8.34}$$

that is, a polynomial weighted by $(1-x^2)^{\frac{1}{2}}$. There is thus an implicit assumption that $f(x)$ vanishes at $x = \pm 1$, and that it possibly has a square-root singularity at these points (though this is not essential).

Now

$$b_i = \frac{2}{n+2} \sum_{k=1}^{n+1} (1-y_k^2)^{\frac{1}{2}} f(y_k) U_i(y_k) \tag{8.35}$$

from (8.33). Integrating (8.18) gives us

$$I_n(f) = \sum_{j=0}^{n} b_j a_j \tag{8.36}$$

where

$$a_j = \int_{-1}^{1} w(x)(1-x^2)^{\frac{1}{2}} U_j(x)\,\mathrm{d}x = \int_0^{\pi} w(\cos\theta)\ \sin(j+1)\theta\ \sin\theta\,\mathrm{d}\theta. \tag{8.37}$$

This gives the rule

$$I_n(f) = \sum_{k=1}^{n+1} w_k f(y_k), \tag{8.38a}$$

$$w_k = (1-y_k^2)^{\frac{1}{2}} \sum_{j=0}^{n} \frac{2a_j}{n+2} U_j(y_k). \tag{8.38b}$$

- In the special case where $w(x) = 1$,

$$a_j = \int_{-1}^{1} (1-x^2)^{\frac{1}{2}} U_j(x)\,\mathrm{d}x = \int_0^{\pi} \sin(j+1)\theta\ \sin\theta\,\mathrm{d}\theta = \begin{cases} \frac{1}{2}\pi, & j = 0, \\ 0, & j > 0. \end{cases}$$

  Hence, from (8.36), (8.37),

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = I_n(f) = \frac{\pi}{n+2} \sum_{k=1}^{n+1} (1-y_k^2)^{\frac{1}{2}} f(y_k). \tag{8.39}$$

This is equivalent to the second-kind Gauss–Chebyshev formula of Theorem 8.4, applied to the function

$$\frac{f(x)}{\sqrt{1-x^2}}.$$

8.3.4 Third-kind formulae

A third-kind formula is obtained from the orthogonality formula

$$d_{ij} = \sum_{k=1}^{n+1}(1+x_k)V_i(x_k)V_j(x_k) = \begin{cases} n+\frac{3}{2}, & i=j, \\ 0, & i \neq j, \end{cases} \tag{8.40}$$

where $\{x_k\}$ are the zeros of $V_{n+1}(x)$. (See Problem 14 of Chapter 4.)

In this case, we choose

$$J_n f(x) = (1+x)^{\frac{1}{2}} \sum_{j=0}^{n} b_j V_j(x), \tag{8.41}$$

a polynomial weighted by $(1+x)^{\frac{1}{2}}$ (implicitly supposing that $f(-1) = 0$). Now, from (8.39), we can show that

$$b_i = \frac{1}{n+\frac{3}{2}} \sum_{k=1}^{n+1}(1+x_k)^{\frac{1}{2}} f(x_k) V_i(x_k). \tag{8.42}$$

Integrating (8.18) gives us again

$$I_n(f) = \sum_{j=0}^{n} b_j a_j$$

where now

$$a_j = \int_{-1}^{1} w(x)(1+x)^{\frac{1}{2}} V_j(x)\,\mathrm{d}x. \tag{8.43}$$

So we have the rule

$$I_n(f) = \sum_{k=1}^{n+1} w_k f(x_k) \tag{8.44a}$$

$$w_k = (1+x_k)^{\frac{1}{2}} \sum_{j=0}^{n} \frac{2a_j}{2n+3} V_j(x_k). \tag{8.44b}$$

- For the special case in which

$$w(x) = (1-x)^{-\frac{1}{2}}, \tag{8.45}$$

then

$$
\begin{aligned}
a_j &= \int_{-1}^{1} (1+x) V_j(x) \frac{\mathrm{d}x}{(1-x^2)^{\frac{1}{2}}} = \\
&= \int_0^{\pi} 2\cos(j+\tfrac{1}{2})\theta \, \cos\tfrac{1}{2}\theta \, \mathrm{d}\theta = \begin{cases} \pi, & j=0, \\ 0, & j>0. \end{cases}
\end{aligned}
$$

Hence

$$
\int_{-1}^{1} f(x) \frac{\mathrm{d}x}{\sqrt{1-x}} = I_n(f) = \frac{2\pi}{2n+3} \sum_{k=1}^{n+1} (1+x_k)^{\frac{1}{2}} f(x_k). \qquad (8.46)
$$

This is equivalent to the third-kind Gauss–Chebyshev formula of Theorem 8.4, applied to the function

$$
\frac{f(x)}{\sqrt{1+x}}.
$$

8.3.5 General remark on methods of Clenshaw–Curtis type

There are effectively two types of quadrature formula considered above.

- For special choices of weight function $w(x)$, such that all but one of the Chebyshev transforms b_i vanish, the formula involves only a single summation — such as (8.27) — and is identical or very similar to a Gauss–Chebyshev formula.

- For a more general weight function, provided that the integral (8.23), (8.37) or (8.43) defining a_j can be exactly evaluated by some means, we obtain a formula involving a double summation — such as (8.24) — one set of summations to compute the weights w_k and a final summation to evaluate the integral.

8.4 Error estimation for Clenshaw–Curtis methods

There are a number of papers on error estimation in Clenshaw–Curtis methods (Fraser & Wilson 1966, O'Hara & Smith 1968, Smith 1982, Favati et al. 1993, for instance). However, we emphasise here the approach of Sloan & Smith (1980), which seems to be particularly robust, depends on interesting properties of Chebyshev polynomials, and is readily extendible to cover all four kinds of Chebyshev polynomial and the plethora of abscissae that were discussed in Section 8.3.

8.4.1 First-kind polynomials

Suppose that the function $f(x)$ being approximated is continuous and of bounded variation, and therefore has a uniformly convergent first-kind Chebyshev expansion

$$f(x) \approx \sum_{j=0}^{\infty}{}' \beta_j T_j(x). \tag{8.47}$$

Then the error in the integration method (8.31) (based on $\{y_k\}$) is

$$\begin{aligned} E_n(f) &:= I(f) - I_n(f) \\ &= (I - I_n)\left(\sum_{j=n+1}^{\infty} \beta_j T_j(x)\right) \\ &= \sum_{j=n+1}^{\infty} \beta_j \{I(T_j) - I_n(T_j)\}. \end{aligned} \tag{8.48}$$

Now

$$I(T_j) = \int_{-1}^{1} w(x) T_j(x)\,\mathrm{d}x = a_j \tag{8.49}$$

and (J_n again denoting the operator interpolating in the points $\{y_k\}$)

$$I_n(T_j) = \int_{-1}^{1} w(x) J_n T_j(x)\,\mathrm{d}x. \tag{8.50}$$

But

$$J_n T_j(y_k) = T_j(y_k) = T_{j'}(y_k) \tag{8.51}$$

where (as shown in Table 8.1) $j' = j'(n, j)$ is an integer in the range $0 \le j' \le n$ defined by

$$\left.\begin{array}{rcll} j'(n,j) &=& j, & 0 \le j \le n \\ j'(n,j) &=& 2n - j, & n \le j \le 2n \\ j'(n, 2n+j) &=& j'(n,j) & \end{array}\right\}. \tag{8.52}$$

This follows immediately from the observation that, j, k and n being integers,

$$T_j(y_k) = \cos\frac{jk\pi}{n} = \cos\frac{(2n \pm j)k\pi}{n} = T_{2n\pm j}(y_k).$$

Thus the interpolation operator J_n has the so-called *aliasing*[1] effect of identifying any Chebyshev polynomial T_j with a polynomial $T_{j'}$ of degree at most n, and it follows from (8.51) that, identically,

$$J_n T_j(x) = T_{j'}(x), \tag{8.53}$$

[1]See Section 6.3.1.

Table 8.1: $T_{j'}(x)$ interpolates $T_j(x)$ in the zeros of $(1-x^2)U_{n-1}(x)$

$j =$	0	1	2	$\rightarrow$	$n-1$	n
	$2n$	$2n-1$	$2n-2$	$\leftarrow$	$n+1$	n
	$2n$	$2n+1$	$2n+2$	$\rightarrow$	$3n-1$	$3n$
	$\vdots$	$\vdots$	$\vdots$		$\vdots$	$\vdots$
$j' =$	0	1	2	$\cdots$	$n-1$	n

and

$$I_n(T_j) = I_n(T_{j'}) = I(T_{j'}) = a_{j'}. \tag{8.54}$$

Therefore

$$E_n(f) = \sum_{j=n+1}^{\infty} \beta_j (a_j - a_{j'}). \tag{8.55}$$

Sloan & Smith (1980) assume that the weight function $w(x)$ is smooth enough for a_j (8.23) to be neglected for $j > 2n$ and that the integrand $f(x)$ itself is smooth enough for β_j (8.47) to be neglected beyond $j = 3n$. Then (8.55) yields, referring to Table 8.1,

$$\begin{aligned} |E_n(f)| \le\ & |a_{n+1} - a_{n-1}|\,|\beta_{n+1}| + |a_{n+2} - a_{n-2}|\,|\beta_{n+2}| + \cdots \\ & \cdots + |a_{2n} - a_0|\,|\beta_{2n}| + |a_1|\,|\beta_{2n+1}| + \cdots + |a_n|\,|\beta_{3n}|\,. \end{aligned}$$

If we then assume a geometric decay in the β_js, say

$$|\beta_{n+j}| \le c_n r_n^j$$

for some c_n, r_n with $r_n < 1$, then

$$|E_n(f)| \le c_n \{ |a_{n+1} - a_{n-1}|\, r_n + \cdots + |a_{2n} - a_0|\, r_n^n + |a_1|\, r_n^{n+1} + \cdots + |a_n|\, r_n^{2n} \}. \tag{8.56}$$

If we change the notation slightly, replacing b_j by b_{nj}, the additional subscript being introduced to show the dependence on n,

$$b_{nj} = \frac{2}{\pi} \sum_{k=0}^{n}{}'' f(y_k) T_j(y_k),$$

it is clear that b_{nj} is an approximation to

$$\beta_j = \frac{2}{\pi} \int_{-1}^{1} f(x) T_j(x) \frac{\mathrm{d}x}{\sqrt{1-x^2}},$$

which becomes increasingly accurate with increasing n. Hence, a succession of values of b_{nj} (for various values of n) may be used to estimate β_j. (For the case $j = n$, β_j would be approximated by $\frac{1}{2} b_{nj}$.)

Sloan and Smith's 'second method' is based on obtaining estimates of r_n and c_n, and then using them in (8.56). Essentially, r_n is estimated from ratios of coefficients and c_n from the coefficients themselves. One algorithm, which takes account of the observed fact that odd and even coefficients tend to have somewhat different behaviours, and which uses three or four coefficients to construct each estimate, is as follows:

- Compute

$$\begin{aligned} z_1 &= \max\{\tfrac{1}{2}\left|b_{nn}\right|, \left|b_{n,n-2}\right|, \left|b_{n,n-4}\right|, \left|b_{n,n-6}\right|\}, \\ z_2 &= \max\{\left|b_{n,n-1}\right|, \left|b_{n,n-3}\right|, \left|b_{n,n-5}\right|. \end{aligned}$$

- If $z_1 > z_2$ then if $\left|b_{n,n-6}\right| > \cdots > \frac{1}{2}\left|b_{nn}\right|$ then

$$r_n^2 = \max\left\{ \frac{\frac{1}{2}\left|b_{nn}\right|}{\left|b_{n,n-2}\right|}, \frac{\left|b_{n,n-2}\right|}{\left|b_{n,n-4}\right|}, \frac{\left|b_{n,n-4}\right|}{\left|b_{n,n-6}\right|} \right\}, \tag{8.57}$$

  otherwise $r_n = 1$.

- If $z_1 < z_2$ then if $\left|b_{n,n-5}\right| > \cdots > \left|b_{n,n-1}\right|$ then

$$r_n^2 = \max\left\{ \frac{\left|b_{n,n-1}\right|}{\left|b_{n,n-3}\right|}, \frac{\left|b_{n,n-3}\right|}{\left|b_{n,n-5}\right|} \right\}, \tag{8.58}$$

  otherwise $r_n = 1$.

- Set

$$c_n = \max\{\tfrac{1}{2}\left|b_{nn}\right|, \left|b_{n,n-1}\right| r_n, \ldots, \left|b_{n,n-6}\right| r_n^6\}. \tag{8.59}$$

8.4.2 Fitting an exponential curve

A similar but somewhat neater procedure for estimating c_n and r_n is to fit the coefficients

$$b_{nn}, b_{n,n-1}, b_{n,n-2}, \ldots, b_{n,n-k}$$

(or the even or odd subsequences of them) by the sequence

$$c_n r_n^n, c_n r_n^{n-1}, c_n r_n^{n-2}, \ldots, c_n r_n^{n-k}.$$

This is in effect a discrete approximation of a function $g(x) = b_{nx}$ by

$$c_n (r_n)^x \equiv \mathrm{e}^{A+Bx}$$

at $x = n, n-1, n-2, \ldots, n-k$, where $A = \ln c_n$ and $B = \ln r_n$.

Then

$$g(x) = \mathrm{e}^{A+Bx} + e(x)$$

where $e(x)$ is the error. Hence

$$\ln g(x) + \ln(1 - e(x)/g(x)) = A + Bx$$

so that, to the first order of approximation,

$$\ln g(x) - e(x)/g(x) \approx A + Bx$$

and

$$g(x)\ln g(x) - e(x) \approx g(x)(A + Bx).$$

Hence a discrete least-squares fit of $\ln g(x)$ by $A+Bx$, weighted throughout by $g(x)$, can be expected to give a good model of the least-squares fitting of $g(x)$ by e^{A+Bx}.

This is an example of an algorithm for approximation by a 'function of a linear form' — more general discussion of such algorithms is given in Mason & Upton (1989).

8.4.3 Other abscissae and polynomials

Analogous procedures to those of Section 8.4.1 can be found for all four kinds of Chebyshev polynomials, and for all sets of abscissae that provide discrete orthogonality.

For example:

- For first-kind polynomials on the zeros $\{x_k\}$ of $T_{n+1}(x)$ (8.24), equations (8.47)–(8.50) still hold, but now

  $$J_n T_j(x_k) = T_j(x_k) = \pm T_{j'}(x_k)$$

  where (as in Table 8.2)

  $$\left.\begin{array}{rcll} j'(n,j) &=& j, & 0 \le j \le n \text{ (with + sign)} \\ j'(n,n+1) &=& n+1 & \text{(with zero coefficient)} \\ j'(n,j) &=& 2n+2-j, & n+2 \le j \le 2n+2 \text{ (} - \text{ sign)} \\ j'(n,j+2n+2) &=& j'(n,j) & \text{(with changed sign)} \end{array}\right\}. \tag{8.60}$$

  This follows immediately from

  $$T_j(x_k) = \begin{cases} \cos\frac{j'(k-\frac{1}{2})\pi}{n+1} & (0 \le j \le n) \\ 0 & (j = n+1) \\ \cos\frac{(2n+2-j')(k-\frac{1}{2})\pi}{n+1} = -\cos\frac{j'(k-\frac{1}{2})\pi}{n+1} & (n+2 \le j \le 2n+2) \\ \cos\frac{(2n+2+j')(k-\frac{1}{2})\pi}{n+1} = -\cos\frac{j'(k-\frac{1}{2})\pi}{n+1} & (2n+3 \le j \le 3n+2) \end{cases}$$

Table 8.2: $\pm T_{j'}(x)$ interpolating $T_j(x)$ in the zeros of $T_{n+1}(x)$

$j =$	0	1	$\rightarrow$	n	$n+1$	$n+2$	$\rightarrow$	$2n+1$	$2n+2$
	$4n+4$	$4n+3$	$\leftarrow$	$3n+4$	$3n+3$	$3n+2$	$\leftarrow$	$2n+3$	$2n+2$
	$4n+4$	$4n+5$	$\rightarrow$	$5n+4$	$5n+5$	$5n+6$	$\rightarrow$	$6n+5$	$6n+6$
	$\vdots$	$\vdots$		$\vdots$	$\vdots$	$\vdots$		$\vdots$	$\vdots$
$j' =$	0	1	$\cdots$	n	$n+1$	n	$\cdots$	1	0
sign	$+$	$+$	$\cdots$	$+$	0	$-$	$\cdots$	$-$	$-$

We now deduce that

$$\begin{aligned} |E_n(f)| \leq\ & |a_{n+1}|\,|\beta_{n+1}| + |a_{n+2} + a_n|\,|\beta_{n+2}| + \cdots \\ & \cdots + |a_{2n+2} + a_0|\,|\beta_{2n+2}| + |a_1|\,|\beta_{2n+3}| + \cdots \\ & \cdots + |a_{n+1}|\,|\beta_{3n+3}|\,. \end{aligned} \tag{8.61}$$

- For second-kind polynomials on the zeros of U_{n+1} (8.38), we require an expansion

$$f(x) = \sum_{j=0}^{\infty} \beta_j U_j(x)$$

so that β_j is approximated by b_j from (8.35).

Then

$$E_n(f) = \sum_{j=n+1}^{\infty} \beta_j [I(U_j) - I_n(U_j)]$$

where now

$$I(U_j) = \int_{-1}^{1} w(x)(1-x^2)^{1/2} U_j(x)\,\mathrm{d}x = a_j \tag{8.62}$$

and

$$I_n(U_j) = \int_{-1}^{1} w(x)(1-x^2)^{1/2} J_n U_j(x)\,\mathrm{d}x. \tag{8.63}$$

If $\{y_k\}$ are the zeros of $U_{n+1}(x)$, then

$$J_n U_j(y_k) = U_j(y_k) = \pm U_{j'}(y_k)$$

where (taking $U_{-1} \equiv 0$)

$$\left.\begin{array}{rcll} j'(n,j) & = & j, & 0 \le j \le n \text{ (with + sign)} \\ j'(n,n+1) & = & n+1 & \text{(with zero coefficient)} \\ j'(n,j) & = & 2n+2-j, & n+2 \le j \le 2n+2 \text{ (} - \text{ sign)} \\ j'(n,2n+3) & = & -1 & \text{(with zero coefficient)} \\ j'(n,j+2n+4) & = & j'(n,j) & \text{(with unchanged sign)} \end{array}\right\}. \tag{8.64}$$

This is shown in Table 8.3, and follows from

$$y_k = \cos\theta_k = \cos\frac{k\pi}{n+2}, \quad k = 1, \ldots, n+1.$$

For

$$\begin{aligned} U_j(y_k)\sin\theta_k &= \sin(j+1)\theta_k \quad (j = 0, \ldots, n) \\ &= \sin(2n+2-j'+1)\theta_k = -\sin(j'+1)\theta_k \\ &= -U_{j'}(y_k)\sin\theta_k \quad (j' = n+1, \ldots) \end{aligned}$$

and

$$\sin(j+2n+4+1)\theta_k = \sin(j+1)\theta_k.$$

Table 8.3: $\pm U_{j'}(x)$ interpolating $U_j(x)$ in the zeros of $U_{n+1}(x)$

$j =$	0	$\to$	n	$n+1$	$n+2$	$\to$	$2n+2$	$2n+3$
	$2n+4$	$\to$	$3n+4$	$3n+5$	$3n+6$	$\to$	$4n+6$	$4n+7$
	$4n+8$	$\to$	$5n+8$	$5n+9$	$5n+10$	$\to$	$6n+10$	$6n+11$
	$\vdots$		$\vdots$	$\vdots$	$\vdots$		$\vdots$	$\vdots$
$j' =$	0	$\cdots$	n	$n+1$	n	$\cdots$	0	-1
sign	$+$	$\cdots$	$+$	0	$-$	$\cdots$	$-$	0

From (8.62) and (8.63):

$$E_n(f) = \sum_{j=n+1}^{\infty} \beta_j (a_j - a_{j'})$$

and

$$\begin{aligned} |E_n(f)| \le\ & |a_{n+1}|\,|\beta_{n+1}| + |a_{n+2} + a_n|\,|\beta_{n+2}| + \cdots \\ & \cdots + |a_{2n+2} + a_0|\,|\beta_{2n+2}| + |a_0|\,|\beta_{2n+4}| + \cdots \\ & \cdots + |a_{n+1}|\,|\beta_{3n+5}|\,. \end{aligned} \tag{8.65}$$

- For third-kind polynomials on the zeros of V_{n+1} (8.44), we use an expansion

$$f(x) = (1+x)^{1/2} \sum_{j=0}^{\infty} \beta_j V_j(x). \tag{8.66}$$

Then

$$E_n(f) = \sum_{j=n+1}^{\infty} \beta_j [I(V_j) - I_n(V_j)]$$

where

$$I(V_j) = \int_{-1}^{1} w(x)(1+x)^{1/2} V_j(x)\,\mathrm{d}x = a_j \tag{8.67}$$

and

$$I_n(V_j) = \int_{-1}^{1} w(x)(1+x)^{1/2} J_n V_j(x)\,\mathrm{d}x. \tag{8.68}$$

Choose $\{x_k\}$ as the zeros of $V_{n+1}(x)$. Then

$$J_n V_j(x_k) = V_j(x_k) = \pm V_{j'}(x_k)$$

where

$$\left.\begin{array}{rcll} j'(n,j) & = & j, & 0 \le j \le n \text{ (with + sign)} \\ j'(n,n+1) & = & n+1 & \text{(with zero coefficient)} \\ j'(n,j) & = & 2n+2-j, & n+2 \le j \le 2n+2 \text{ ($-$ sign)} \\ j'(n,j+2n+3) & = & j'(n,j) & \text{(with changed sign)} \end{array}\right\}. \tag{8.69}$$

This is shown in Table 8.4, and follows from

$$x_k = \cos\theta_k = \cos\frac{(k-\frac{1}{2})\pi}{n+\frac{3}{2}},$$

giving

$$\begin{aligned} \cos\tfrac{1}{2}\theta_k V_j(x_k) &= \cos\frac{(j+\frac{1}{2})(k-\frac{1}{2})\pi}{n+\frac{3}{2}} \\ &= \cos\frac{(2n+2-j'+\frac{1}{2})(k-\frac{1}{2})\pi}{n+\frac{3}{2}} \\ &= \cos\frac{\{2(n+\frac{3}{2})-(j'+\frac{1}{2})\}(k-\frac{1}{2})\pi}{n+\frac{3}{2}} \\ &= -\cos\frac{(j'+\frac{1}{2})(k-\frac{1}{2})\pi}{n+\frac{3}{2}} \end{aligned}$$

and

$$\cos\frac{(j+2n+3+\frac{1}{2})(k-\frac{1}{2})\pi}{n+\frac{3}{2}} = -\cos\frac{(j+\frac{1}{2})(k-\frac{1}{2})\pi}{n+\frac{3}{2}}.$$

Table 8.4: $\pm V_{j'}(x)$ interpolating $V_j(x)$ in the zeros of $V_{n+1}(x)$

$j =$	0	$\rightarrow$	n	$n+1$	$n+2$	$\rightarrow$	$2n+2$
	$4n+5$	$\leftarrow$	$3n+5$	$3n+4$	$3n+3$	$\leftarrow$	$2n+3$
	$4n+6$	$\rightarrow$	$5n+6$	$5n+7$	$5n+8$	$\rightarrow$	$6n+8$
	$\vdots$		$\vdots$	$\vdots$	$\vdots$		$\vdots$
$j' =$	0	$\cdots$	n	$n+1$	n	$\cdots$	0
sign	$+$	$\cdots$	$+$	0	$-$	$\cdots$	$-$

From (8.67) and (8.68):

$$E_n(f) = \sum_{j=n+1}^{\infty} \beta_j (a_j - a_{j'})$$

and

$$\begin{aligned} |E_n(f)| \le\ & |a_{n+1}|\,|\beta_{n+1}| + |a_{n+2} + a_n|\,|\beta_{n+2}| + \cdots \\ & \cdots + |a_{2n+2} + a_0|\,|\beta_{2n}| + |a_0|\,|\beta_{2n+3}| + \cdots \\ & \cdots + |a_n|\,|\beta_{3n+3}|\,. \end{aligned} \tag{8.70}$$

We note that there are only very slight differences between Tables 8.2, 8.3 and 8.4 and between the corresponding error bounds (8.61), (8.65) and (8.70).

8.5 Some other work on Clenshaw–Curtis methods

There is now a significant amount of literature on Clenshaw–Curtis methods, built up over about forty years, from which we shall draw attention to a selection of items.

Of particular interest are applications to Bessel function integrals (Piessens & Branders 1983), oscillatory integrals (Adam 1987), Fourier transforms of singular functions (Piessens & Branders 1992), Cauchy principal-value integrals (Hasegawa & Torii 1991) and Volterra integral equations (Evans et al. 1981).

Among contributions specific to error bounds and error estimates are the early work of Chawla (1968), Locher (1969) and O'Hara & Smith (1968), together with more recent work of Smith (1982) and Favati et al. (1993)—the last being concerned with analytic functions.

Product integration (including error estimation) has been well studied, in particular by Sloan & Smith (1978, 1980, 1982) and Smith & Paget (1992).

There has been an important extension of the Clenshaw–Curtis method to integration over a d-dimensional hypercube, by Novak & Ritter (1996).

8.6 Problems for Chapter 8

1. If $w = (1-x^2)^{-\frac{1}{2}}$ and $P_k(x) = T_k(x)$ in Section 8.1, show that

$$\begin{aligned} \|h - h_n\|_\infty &= \int_{-1}^{1} (1-x^2)^{-\frac{1}{2}} \left| f(x) - \sum_{k=0}^{n}{}' a_k T_k(x) \right| \mathrm{d}x \\ &= \int_0^\pi \left| f(\cos\theta) - \sum_{k=0}^{n}{}' a_k \cos k\theta \right| \mathrm{d}\theta. \end{aligned}$$

   By considering the Fourier cosine series expansion of $f(\cos\theta)$, deduce Theorem 8.1 for the first case.

2. If $w = [\frac{1}{2}(1-x)]^{-\frac{1}{2}}$ and $P_k(x) = V_k(x)$ in Section 8.1, show that

$$\begin{aligned} \|h - h_n\|_\infty &= \int_{-1}^{1} [\tfrac{1}{2}(1-x)]^{-\frac{1}{2}} \left| f(x) - \sum_{k=0}^{n} a_k V_k(x) \right| \mathrm{d}x \\ &= 2\int_0^\pi \left| \cos\tfrac{1}{2}\theta\, f(\cos\theta) - \sum_{k=0}^{n} a_k \cos(k+\tfrac{1}{2})\theta \right| \mathrm{d}\theta \\ &= 4\int_0^{\pi/2} \left| \cos\phi\, f(\cos 2\phi) - \sum_{k=0}^{n} a_k \cos(2k+1)\phi \right| \mathrm{d}\phi. \end{aligned}$$

   By considering the Fourier cosine series expansion of $\cos\phi\, f(\cos 2\phi)$ (which is odd about $\phi = \frac{1}{2}\pi$), deduce Theorem 8.1 for the third case.

3. Complete the proof of Lemma 8.3, by performing an induction on n for the pair of formulae together.

4. Use Lemma 8.3 to prove the second part of Theorem 8.4. Verify that this quadrature formula is exact for $n = 3$ in the case of the integral

$$\int_{-1}^{1} \sqrt{1-x^2}\, x^2 \,\mathrm{d}x.$$

5. Prove in detail the second part of Lemma 8.5.

6. Verify the exactness of Gauss–Chebyshev quadrature using first-kind polynomials, by testing it for $n = 4$ and $f(x) = x^6$, $f(x) = x^7$.

7. Verify the Gauss–Chebyshev rule for fourth-kind polynomials, by testing it for $n = 1$ and $f(x) = 1$, $f(x) = x$.

8. Verify that there is a Gauss–Chebyshev quadrature rule based on the zeros of $(1-x^2)U_{n-1}(x)$ and the polynomials $T_n(x)$, and derive a formula. (This type of formula, which uses both end points, is called a *Lobatto* rule.) When would this rule be useful?

9. Show that there is a Gauss–Chebyshev quadrature rule based on the zeros of $(1+x)V_n(x)$ and the polynomials $T_n(x)$, and derive a formula. (This type of formula, which uses one end point, is called a *Radau* rule.) When would this rule be useful?