TABLE 6.2

$T_{0,i}$	$T_{1,i}$	$T_{2,i}$	$T_{3,i}$
0.92073549			
0.93979328	0.94614588		
0.94451352	0.94608693	0.94608300	
0.94569086	0.94608331	0.94608307	0.94608307

PROBLEMS, SECTION 6.4.1

1. Repeat Example 6.7 for $f(x) = \sqrt{x}$; estimate $f'(2)$ with $h = .8$ and $r = 1/2$.
2. Use Richardson extrapolation to estimate $f'(x)$ at $x = 1$ where $f(x) = \ln(x)$. In Table 6.1, use $n = 4$ and $h = 0.4$ and $r =$. Try both forms of $A(h)$: the form given in Example 6.6 and that given in Example 6.7.
3. Show that formula (6.28) is valid by writing down the Taylor's series expansion for $f(x + h)$ and $f(x - h)$ and expanding about $x = \alpha$ in both cases.
4. Verify the expansion in (6.29).
5. Write a computer program to carry out Romberg integration; test your program on the Fresnel integral given in Problem 3, Section 6.3. To determine (in a rough fashion) the accuracy of your answers, print out the ratios defined in (6.33).
6. The fundamental assumption of Richardson extrapolation can be seen from (6.21). We are assuming that $a_0 - A(h) = a_k h^k + a_{k+1}h^{k+1} + \cdots$ and that eliminating $a_k h^k$ will lead to a better approximation. That is, we are assuming that $a_k h^k$ is the dominant term in the error $a_0 - A(h)$.
   a) Show that the assumption above means that the ratio
   $$[A_{0,m} - A_{0,m-1}]/[A_{0,m+1} - A_{0,m}]$$
   should be approximately r^{-k}.
   b) Use part (a) to establish that the ratios $R_{i,m}$ defined in (6.33) should be approximately 4^{i+1} if Romberg integration is proceeding without a substantial error.
7. Calculate the appropriate ratios, as defined in Problem 6, for the tables in Examples 6.7 and 6.8.
8. Show that $T_{1,m}$ defined in (6.32) corresponds to the composite Simpson's rule. (However, there is no relation between $T_{k,m}$ and Newton-Cotes rules for $k > 2$.)

6.5 GAUSSIAN QUADRATURE

As we previously remarked in Section 6.2, if we let the quadrature weights, $\{A_j\}_{j=0}^n$, *and* the quadrature nodes, $\{x_j\}_{j=0}^n$, be treated as unknown variables, then the equations of (6.3),

$$\int_a^b x^k w(x)\,dx = \sum_{j=0}^n A_j x_j^k, \qquad 0 \le k \le 2n + 1, \tag{6.34}$$

represent a nonlinear system of $(2n + 2)$ equations in $(2n + 2)$ unknowns. In 1814, Gauss was able to show that this system of equations has a unique solution for the unknowns $\{A_j\}_{j=0}^n$ and $\{x_j\}_{j=0}^n$ when $w(x) \equiv 1$ and $[a, b] = [-1, 1]$.

Once again we return to the notation of Section 5.3, in which we let $\langle f, g\rangle \equiv \int_a^b f(x)g(x)w(x)\,dx$, and $\|f\| \equiv \langle f, f\rangle^{1/2}$. We let $\{q_j(x)\}_{j=0}^\infty$ denote the *monic* orthogonal polynomials and $\{p_j(x)\}_{j=0}^\infty$ the orthonormal polynomials with respect to this inner product where degree $(q_j(x))$ = degree $(p_j(x)) = j$ for each j. We first prove the following theorem, which localizes the zeros of each $p_j(x)$. [Recall that for each j, $p_j(x)$ is a constant multiple of $q_j(x)$; and thus they have the same zeros.]

Theorem 6.3

Let $\{p_j(x)\}_{j=0}^\infty$ be given as above. Then for each $n \geq 1$, the zeros of $p_n(x)$ are real and distinct and lie in the interval (a, b).

Proof. Let $n \geq 1$ be fixed and suppose that none of the zeros of $p_n(x)$ are in (a, b) so that $p_n(x)$ is of constant sign on (a, b) [say $p(x) > 0$ for $x \in (a, b)$]. By the orthogonality of $p_n(x)$ and $q_0(x)$, $(q_0(x) \equiv 1)$, we would then have

$$0 = \langle 1, p_n\rangle = \int_a^b p_n(x)w(x)\,dx > 0$$

since we assume $w(x)$ is nonnegative and strictly positive for some subinterval of (a, b). Thus our initial assumption is contradicted, and $p_n(x)$ must have at least one zero, x_0, in (a, b).

If any zero, say x_0, is a multiple zero of $p_n(x)$, then $(x - x_0)^2$ factors $p_n(x)$ and so $r(x) \equiv p_n(x)/(x - x_0)^2$ is in $\mathcal{P}_{n-2}$. By Corollary 1 of Theorem 5.9, $\langle p_n, r\rangle = 0$; and so we can write

$$0 = \langle p_n, r\rangle = \int_a^b p_n(x)[p_n(x)/(x - x_0)^2]w(x)\,dx$$

$$= \int_a^b \frac{p_n(x)^2}{(x - x_0)^2} w(x)\,dx > 0,$$

which is again a contradiction. Hence we can infer that any zero of $p_n(x)$ lying in (a, b) is simple.

Now let $\{x_0, x_1, \ldots, x_j\}$ be the zeros of $p_n(x)$ lying in (a, b); and suppose that $j < n - 1$; that is, $p_n(x)$ has other zeros elsewhere. Since the zeros $\{x_i\}_{i=0}^j$ are simple, we can form the polynomial $p_n(x)[(x - x_0)(x - x_1) \cdots (x -$

$x_j)]$. We write this polynomial as $r(x) \cdot [(x - x_0)^2(x - x_1)^2 \cdots (x - x_j)^2]$ where $r(x) \in \mathcal{P}_{n-j-1}$, and we note that $r(x)$ is of constant sign (say >0) on (a, b). Again

$$\langle p_n(x), [(x - x_0)(x - x_1) \cdots (x - x_j)] \rangle = 0$$

by the corollary mentioned above. So

$$0 = \int_a^b p_n(x)[(x - x_0)(x - x_1) \cdots (x - x_j)]w(x)\, dx$$

$$= \int_a^b r(x)[(x - x_0)^2(x - x_1)^2 \cdots (x - x_j)^2]w(x)\, dx > 0,$$

which contradicts the assumption that $j < n - 1$. Thus all the zeros of $p_n(x)$ are in (a, b) and are simple. ■

Recall that the Eqs. (6.34) are satisfied for $0 \le k \le 2n + 1$ if and only if $Q_n(f) = \Sigma_{j=0}^n A_j f(x_j)$ has precision $2n + 1$; that is, if $f(x)$ is any polynomial of degree $(2n + 1)$ or less, then $I(f) = Q_n(f)$. (Any interpolatory quadrature formula with this property is called *Gaussian*.) With this point in mind we are able to prove the basic theorem of Gaussian quadrature.

Theorem 6.4

The formula $\int_a^b p(x)w(x)\, dx = \Sigma_{j=0}^n A_j p(x_j)$ holds for all $p(x)$ in $\mathcal{P}_{2n+1}$ if and only if $\{x_j\}_{j=0}^n$ are the zeros of $p_{n+1}(x)$ (as given in Theorem 6.3) and $\{A_j\}_{j=0}^n$ are given in (6.2).

Proof. 1. Let $p(x) \in \mathcal{P}_{2n+1}$ and let $p_{n+1}(x_j) = 0$, $0 \le j \le n$. By the Euclidean division algorithm, $p(x)$ can be written as $p(x) = p_{n+1}(x)S(x) + R(x)$ where $S(x)$ and $R(x)$ are in $\mathcal{P}_n$. [Note that since $p_{n+1}(x_j) = 0$, $0 \le j \le n$, then $p(x_j) = R(x_j)$, $0 \le j \le n$.] In addition, since the weights are given by (6.2), $I(R) = Q_n(R) = \Sigma_{j=0}^n A_j R(x_j)$ (since the quadrature formula has precision at least n). If one uses Corollary 1 of Theorem 5.9, $\langle p_{n+1}, S \rangle = 0$; so

$$I(p) \equiv \int_a^b p(x)w(x)\, dx = \int_a^b p_{n+1}(x)S(x)w(x)\, dx + \int_a^b R(x)w(x)\, dx$$

$$= \langle p_{n+1}, S \rangle + I(R) = 0 + \sum_{j=0}^n A_j R(x_j)$$

$$= \sum_{j=0}^n A_j p(x_j) = Q_n(p).$$

2. Now we assume that $\{x_j\}_{j=0}^n$ is any distinct set of points and $\int_a^b p(x)w(x)\, dx = \Sigma_{j=0}^n A_j p(x_j)$ for all $p(x) \in \mathcal{P}_{2n+1}$. Given any integer k, $0 \le k \le n$, let $r_k(x)$ be any polynomial of degree k or less. Let $W(x) = \Pi_{j=0}^n (x - x_j)$ and define $p(x) \equiv$

$r_k(x)W(x)$. Then $p(x) \in \mathcal{P}_{2n+1}$; and by our hypothesis, $I(p) = Q_n(p)$. Using this equality, we have

$$\langle r_k, W\rangle = \int_a^b r_k(x)W(x)w(x)\,dx = \int_a^b p(x)w(x)\,dx$$

$$= \sum_{j=0}^{n} A_j p(x_j) = \sum_{j=0}^{n} A_j r_k(x_j)W(x_j) = 0$$

since $W(x_j) = 0$, $0 \le j \le n$. Hence we have just shown that $W(x)$, a monic polynomial of degree $(n + 1)$, is orthogonal to any polynomial of degree n or less. By Corollary 2, Theorem 5.9, $W(x) \equiv q_{n+1}(x)$; and thus x_j's are the zeros of $p_{n+1}(x)$. Now that the nodes x_j are known, we are nearly done. That the weights A_j are as in (6.2) follows immediately since the first $(n + 1)$ equations on the right-hand side of (6.34) constitute a linear system where the coefficient matrix is Vandermonde. Hence there is one and only one choice for the weights, and (6.2) gives the solution explicitly. ■

Gaussian quadratures are powerful numerical integration methods as the following corollary illustrates.

Corollary

Let $Q_n(f) = \sum_{j=0}^{n} A_j f(x_j)$ be Gaussian; then $\lim_{n\to\infty} Q_n(f) = I(f)$ for all $f(x) \in C[a, b]$.

Proof. By the definition of $\ell_k(x)$ [(5.2) in Chapter 5], for each k, $(\ell_k(x))^2 \in \mathcal{P}_{2n}$; and so $I(\ell_k^2) = Q_n(\ell_k^2)$. Thus

$$0 < \int_a^b (\ell_k(x))^2 w(x)\,dx = \sum_{j=0}^{n} A_j(\ell_k(x_j))^2 = A_k$$

since $(\ell_k(x_j))^2 = \delta_{jk}$. Thus the Gaussian quadrature weights are positive for each n; so by the remarks following Theorem 6.1 this corollary is proved. ■

We should also note that since this corollary shows that the weights are all positive, the formulas have nice rounding properties. In the literature there exist extensive tables for the weights and nodes of many common Gaussian quadratures. [For example, see Stroud and Secrest (1966).] We shall now consider efficient methods for calculating the weights and nodes of any Gaussian formula.

To compute the nodes we take the obvious course of generating $q_{n+1}(x)$ by the three-term recurrence formula, (5.65). Since the zeros of $q_{n+1}(x)$ are simple and lie in (a, b), Newton's method is ideally suited for computing these nodes.

Efficient computation of the weights is not so straightforward. We could use the computed values for the nodes and solve for the weights by formula (6.3) or we could use the formula $A_j = \int_a^b \ell_j(x)w(x)\,dx$, $0 \le j \le n$. There is a more efficient procedure, however, which uses the same recurrence relation as for $q_{n+1}(x)$, but has *different starting values* (otherwise we would be just generating the $q_j(x)$'s again).

We first define a new sequence of polynomials, $\{\phi_0, \phi_1, \phi_2, \ldots, \phi_{n+1}\}$, by $\phi_0(x) \equiv 0$, $\phi_1(x) \equiv \int_a^b w(x)\,dx$, and

$$\phi_k(x) = (x - a_k)\phi_{k-1}(x) - b_k\phi_{k-2}(x) \qquad \text{for } k \geq 2. \tag{6.35}$$

The constants $\{a_k\}_{k=2}^{n+1}$ and $\{b_k\}_{k=2}^{n+1}$ are the same as in (5.65), the three-term recurrence that we have just used to find $q_{n+1}(x)$ in order to compute the nodes. [The reader should note that $\phi_0(x)$ and $\phi_1(x)$ differ from $q_0(x)$ and $q_1(x)$, respectively. One should also note that the degree of $\phi_j(x)$ is $j - 1$.] We have introduced (6.35) so that we can calculate each A_j by

$$A_j = \phi_{n+1}(x_j)/q'_{n+1}(x_j), \qquad 0 \leq j \leq n. \tag{6.36}$$

The validity of (6.36) is an immediate consequence of the following theorem.

Theorem 6.5

Let $\phi_{n+1}(x)$ and $q_{n+1}(x)$ be generated by (6.35) and (5.65), respectively. Then $\phi_{n+1}(x)$ can alternatively be written as

$$\phi_{n+1}(x) = \int_a^b \frac{q_{n+1}(t) - q_{n+1}(x)}{(t - x)}\, w(t)\,dt. \tag{6.37}$$

Proof. The proof is by induction and we leave to the reader to verify (6.37) for $n = -1$ and $n = 0$. Then for $n \geq 1$, assume (6.37) is valid for all positive integers up to n. By the three-term recurrence, (5.65),

$$\int_a^b \frac{q_{n+1}(t) - q_{n+1}(x)}{(t - x)}\, w(t)\,dt$$

$$= \int_a^b \frac{[(t - a_{n+1})q_n(t) - b_{n+1}q_{n-1}(t) - (x - a_{n+1})q_n(x) + b_{n+1}q_{n-1}(x)]w(t)\,dt}{(t - x)}.$$

Adding and subtracting $xq_n(t)$ from the numerator of the integrand and recalling that $\int_a^b q_n(t)w(t)\,dt = 0$ reduce this expression to

$$(x - a_{n+1}) \int_a^b \frac{q_n(t) - q_n(x)}{t - x}\, w(t)\,dt - b_{n+1} \int_a^b \frac{q_{n-1}(t) - q_{n-1}(x)}{t - x}\, w(t)\,dt$$

$$+ \int_a^b q_n(t)w(t)\,dt = (x - a_{n+1})\phi_n(x) - b_{n+1}\phi_{n-1}(x) = \phi_{n+1}(x). \qquad \blacksquare$$

To see that (6.36) follows from this theorem, note that $\ell_j(x)$ can alternatively be written as $\ell_j(x) = q_{n+1}(x)/[(x - x_j)q'_{n+1}(x_j)]$, $0 \le j \le n$. Thus since $q_{n+1}(x_j) = 0$ and $q'_{n+1}(x_j) \neq 0$ (by Theorem 6.3), (6.37) yields

$$\frac{\phi_{n+1}(x_j)}{q'_{n+1}(x_j)} = \int_a^b \frac{q_{n+1}(t) - 0}{(t - x_j)q'_{n+1}(x_j)} w(t)\, dt = \int_a^b \ell_j(t)w(t)\, dt \equiv A_j.$$

EXAMPLE 6.9. We pause here to present a particularly nice type of Gaussian quadrature since we can derive closed-form formulas for its weights and nodes for any n. If we let $\langle f, g\rangle = \int_{-1}^{1} f(x)g(x)(1 - x^2)^{-1/2}\, dx$, then the orthogonal polynomials are the Chebyshev polynomials of the first kind, $T_k(x) = \cos[k \cos^{-1}(x)]$. Thus we immediately have the nodes since the zeros of $T_{n+1}(x)$ are $x_j = \cos((2j + 1)\pi/(2n + 2))$, $0 \le j \le n$. To find the weights, we must introduce the Chebyshev polynomials of the second kind, $U_k(x) \equiv \sin[(k + 1)\cos^{-1}(x)]/\sin[\cos^{-1}(x)]$, or $U_k(cos(\theta)) = \sin[(k + 1)\theta]/\sin(\theta)$ for $x \equiv \cos(\theta)$. Now obviously $U_0(x) \equiv 1$ and $U_1(x) = U_1(\cos(\theta)) = \sin(2\theta)/\sin(\theta) = 2\cos(\theta) = 2x$. By elementary trigonometric identities we can show that

$$\sin[(k + 2)\theta] = 2\cos(\theta)\sin[(k + 1)\theta] - \sin(k\theta);$$

and so for $k \ge 1$,

$$\begin{aligned} U_{k+1}(x) \equiv U_{k+1}(\cos(\theta)) &\equiv \sin[(k + 2)\theta]/\sin(\theta) \\ &= 2\cos(\theta)\sin[(k + 1)\theta]/\sin(\theta) - \sin(k\theta)/\sin(\theta) \\ &= 2\cos(\theta)U_k(\cos(\theta)) - U_{k-1}(\cos(\theta)) = 2xU_k(x) - U_{k-1}(x). \end{aligned} \tag{6.38a}$$

Formula (6.38a) shows that $U_k(x)$ is a polynomial of degree k with leading coefficient 2^k [since $U_0(x) \equiv 1$ and $U_1(x) = 2x$]. Thus $V_k(x) \equiv 2^{-k}U_k(x)$ is monic in $\mathcal{P}_k$ and by (6.38a) satisfies the recurrence formula $V_0(x) = 1$, $V_1(x) = x$,

$$V_k(x) = xV_{k-1}(x) - \frac{1}{4}V_{k-2}(x), \qquad k \ge 2. \tag{6.38b}$$

Similarly the monic Chebyshev polynomial of the first kind, $q_k(x) \equiv T_k(x)/2^{k-1}$, $k \ge 1$, satisfies (Problem 4)

$$q_k(x) = xq_{k-1}(x) - b_k q_{k-2}(x), \qquad k \ge 2,$$

where $b_2 = 1/2$ and $b_k = 1/4$ for $k \ge 3$. [This result follows from $T_0(x) = 1$, $T_1(x) = x$, and $T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x)$, $k \ge 2$.]

Now to use (6.36), we must find $\phi_{n+1}(x)$ from (6.35). We have $\phi_0(x) \equiv 0$, $\phi_1(x) = \int_{-1}^{1} (1 - x^2)^{-1/2}\, dx = \pi$, and $\phi_k(x) = x\phi_{k-1}(x) - b_k\phi_{k-2}(x)$, $k \ge 2$. If $k = 2$, $\phi_2(x) = x(\pi) - b_2(0) = \pi x$. If $k = 3$, $\phi_3(x) = \pi x^2 - \pi/4 = \pi V_2(x)$. Since $\phi_2(x) = \pi V_1(x)$ and for $k > 3$ (6.35) is $\phi_k(x) = x\phi_{k-1}(x) - \phi_{k-2}(x)/4$, we see by (6.38b) that $\phi_{k+1}(x) = \pi V_k(x)$, $k \ge 0$. Hence $\phi_{n+1}(x) = \pi V_n(x) = \pi 2^{-n}U_n(x)$. Now

$$\frac{d}{dx}(T_{n+1}(x)) = \frac{d(\cos[(n + 1)\theta])}{d\theta}\frac{d\theta}{dx} = (n + 1)\frac{\sin[(n + 1)\theta]}{\sin(\theta)} = (n + 1)U_n(x).$$

Thus (6.36) becomes

$$A_j = \frac{\phi_{n+1}(x_j)}{q'_{n+1}(x_j)} = \frac{\pi 2^{-n}U_n(x_j)}{(n + 1)2^{-n}U_n(x_j)} = \frac{\pi}{(n + 1)}, \qquad 0 \le j \le n.$$

This equation yields the Gaussian formula

$$\int_{-1}^{1} f(x)(1 - x^2)^{-1/2}\,dx \approx \frac{\pi}{n+1}\sum_{j=0}^{n} f(x_j). \tag{6.39}$$

This particular Gaussian quadrature is called a *Gauss-Chebyshev* quadrature and has especially nice rounding characteristics since the weights are all equal.

Perhaps the most commonly used Gaussian quadrature is obtained from $w(x) \equiv 1$ and $\langle f, g\rangle = \int_{-1}^{1} f(x)g(x)\,dx$. The orthogonal polynomials for this case are the Legendre polynomials. There are no nice closed-form formulas for the nodes and the weights in this case. However, with the use of extensive previously tabulated results and our ability to translate easily the integral of integration from $[-1, 1]$ to $[a, b]$, this quadrature (called a *Gauss-Legendre* quadrature or sometimes even simply a *Gauss quadrature*) is a very practical tool.

If $f(x) \in C^{(2n+2)}[a, b]$, then it is possible to derive an error formula for Gaussian quadrature of this form (see Ralston, 1965):

$$R_n(f) \equiv I(f) - Q_n(f) = \frac{f^{(2n+2)}(\eta)}{(2n+2)!}\int_a^b (q_{n+1}(x))^2 w(x)\,dx. \tag{6.40a}$$

We shall take a slightly different approach that emphasizes the benefits of having precision $(2n + 1)$. Once again, we define the uniform degree of approximation as

$$E_m(f) = \min_{p(x)\in\mathcal{P}_m}\left\{\max_{a\le x\le b}|f(x) - p(x)|\right\} = \min_{p(x)\in\mathcal{P}_m}\{\|f - p\|_\infty\} \equiv \|f - p_m^*\|_\infty.$$

Since $I(1) = Q_n(1)$ for any Gaussian formula, we have $\int_a^b w(x)\,dx = \sum_{j=0}^{n} A_j$. Since the formula is Gaussian, $A_j \ge 0$, $0 \le j \le n$, and $I(p) = Q_n(p)$ for all $p(x) \in \mathcal{P}_{2n+1}$. Thus if $p_{2n+1}^*(x) \in \mathcal{P}_{2n+1}$ is the best uniform polynomial approximation to $f(x)$,

$$\begin{aligned} R_n(f) &\equiv I(f) - Q_n(f) = (I(f) - I(p_{2n+1}^*)) - (Q_n(f) - Q_n(p_{2n+1}^*)) \\ &= \int_a^b (f(x) - p_{2n+1}^*(x))w(x)\,dx - \sum_{j=0}^{n} A_j(f(x_j) - p_{2n+1}^*(x_j)). \end{aligned}$$

Therefore

$$|R_n(f)| \le E_{2n+1}(f)\left(\int_a^b w(x)\,dx + \sum_{j=0}^{n} A_j\right) = 2E_{2n+1}(f)\int_a^b w(x)\,dx. \tag{6.40b}$$

Obviously if any interpolatory quadrature, $Q_n(f) = \sum_{j=0}^{n} B_j f(x_j)$, has precision m and $B_j \ge 0$, $0 \le j \le n$, the argument above could be repeated to yield $|R_n(f)| \le 2E_m(f)\int_a^b w(x)\,dx$. Since the precision is maximized when the quadrature is Gaussian, that is, $m = 2n + 1$, and since $E_{2n+1}(f) \le E_m(f)$ for $m < 2n + 1$, then (6.40b) represents an optimal error bound of this type. For practical use of (6.40b) we can call on any Jackson theorem [for instance, (5.69a) or

(5.69b)] to yield a fairly simple bound on $|R_n(f)|$. We also note (Problem 6) that no formula of the type (6.34) can have precision equal to $2n + 2$. Thus Gaussian formulas are the outside limits in increasing precision.

EXAMPLE 6.10. As an illustration of the power of Gauss-Legendre quadrature, we consider again

$$Si(1) = \int_0^1 \frac{\sin(t)}{t}\,dt.$$

From a table, we obtain the weights and nodes for the five-point Gauss-Legendre formula for $[-1, 1]$:

$$\begin{array}{ll} x_0 = -0.9061798459 & A_0 = 0.2369268851 \\ x_1 = -0.5384693101 & A_1 = 0.4786286705 \\ x_2 = 0.0 & A_2 = 0.5688888889 \\ x_3 = 0.5384693101 & A_3 = 0.4786286705 \\ x_4 = 0.9061798459 & A_4 = 0.2369268851. \end{array}$$

[The symmetric character of the weights and the nodes should be expected since the nth degree Legendre polynomials is an even function when n is even and an odd function when n is odd.] Since our problem is to estimate an integral on $[0, 1]$ rather than on $[-1, 1]$, we must use (6.4) where $a = 0$ and $b = 1$. With this change, the Gauss-Legendre five-point formula provides the estimate of 0.94608307, which is correct to eight places.

6.5.1. Interpolation at the Zeros of Orthogonal Polynomials

Gaussian quadrature provides a valuable link between the integral inner product, $\langle f, g\rangle \equiv \int_a^b f(x)g(x)w(x)\,dx$, and the discrete inner product,

$$\langle f, g\rangle_d = \sum_{j=0}^{n} A_j f(x_j)g(x_j),$$

where A_j and x_j, $0 \le j \le n$, are the weights and the nodes respectively of the Gaussian quadrature $Q_n(f) \approx \int_a^b f(x)w(x)\,dx$. [Note that since the quadrature is Gaussian, then $A_j. > 0$ and $x_j \in (a, b)$, $0 \le j \le n$, so that $\langle f, g\rangle_d$ is a well-defined discrete inner product.]

Theorem 6.6

Given $\langle f, g\rangle$ and $\langle f, g\rangle_d$ as above, let $\{p_0(x), p_1(x), p_2(x), \ldots\}$ be orthonormal polynomials [with degree $(p_j(x)) = j$] with respect to $\langle f, g\rangle$. Then $\{p_0(x), p_1(x), \ldots, p_n(x)\}$ is an orthonormal set with respect to $\langle f, g\rangle_d$.

Proof. Let $p(x) \equiv p_k(x)p_m(x)$, $k + m \le 2n$. Then since $I(p) = Q_n(p)$, we have

$$\delta_{km} = \langle p_k, p_m\rangle = \int_a^b p_k(x)p_m(x)w(x)\,dx = I(p) = Q_n(p)$$

$$= \sum_{j=0}^{n} A_j p_k(x_j)p_m(x_j) = \langle p_k, p_m\rangle_d. \qquad \blacksquare$$

We can use Theorem 6.6 to give an easily computable formula for the polynomial, $P(x) \in \mathcal{P}_n$, that interpolates a function, $f(x)$, at the zeros of $p_{n+1}(x)$.

Theorem 6.7

Let $\{x_j\}_{j=0}^n$ be the zeros of $p_{n+1}(x)$ (as in Theorem 6.6), and let $P(x) = \Sigma_{k=0}^n \alpha_k p_k(x)$. If $\alpha_k = \Sigma_{j=0}^n A_j p_k(x_j) f(x_j)$, then $P(x_j) = f(x_j)$ for $0 \le j \le n$.

Proof. From Chapter 5 we know that the interpolating polynomial exists, is unique, and thus can be written in the form $P(x) = \Sigma_{k=0}^n \alpha_k p_k(x)$. If $P(x_j) = f(x_j)$, then $\Sigma_{k=0}^n \alpha_k p_k(x_j) = f(x_j)$, $0 \le j \le n$. Now for m fixed, multiplying both sides by $A_j p_m(x_j)$ and summing from $j = 0$ to $j = n$ yield

$$\sum_{j=0}^{n} A_j p_m(x_j) f(x_j) = \sum_{j=0}^{n} \left(A_j p_m(x_j) \sum_{k=0}^{n} \alpha_k p_k(x_j) \right)$$

$$= \sum_{k=0}^{n} \alpha_k \left(\sum_{j=0}^{n} A_j p_m(x_j) p_k(x_j) \right) = \sum_{k=0}^{n} \alpha_k \langle p_m, p_k \rangle_d = \alpha_m.$$

This equality holds for each m, $0 \le m \le n$, and so the proof is complete. ■

We next turn our attention to an estimate of the error that is made when interpolating at the zeros of orthogonal polynomials. Suppose $p(x) \in \mathcal{P}_n$ interpolates $f(x)$, $f^{(n+1)}(x) \in C[a, b]$, at *any* set of $(n + 1)$ distinct points, $\{z_j\}_{j=0}^n$, in $[a, b]$. Then we recall from formula (5.27) that for any $x \in [a, b]$

$$f(x) - p(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} W(x) \tag{6.41a}$$

where $\xi \in \text{Spr}\{x, z_0, z_1, \ldots, z_n\}$ and where $W(x) = \Pi_{j=0}^n (x - z_j)$. We have already seen the merits of interpolating at the zeros of the shifted Chebyshev polynomials, $\tilde{T}_{n+1}(x)$, in that this minimizes $\|W\|_\infty \equiv \max_{a \le x \le b} |W(x)|$ [see formula (5.35)]. There are similar advantages in the interpolation given in Theorem 6.7. Recall, as in (5.31), if we square both sides of (6.41a), multiply by $w(x)$, integrate from a to b, and take the square root, we have

$$\begin{aligned} \|f - p\| &= \left(\int_a^b (f(x) - p(x))^2 w(x)\, dx \right)^{1/2} \\ &\le \frac{\max_{a \le x \le b} |f^{(n+1)}(x)|}{(n+1)!} \left(\int_a^b (W(x))^2 w(x)\, dx \right)^{1/2} \\ &= \frac{\|f^{(n+1)}\|_\infty}{(n+1)!} \|W\|. \end{aligned} \tag{6.41b}$$

Now let $W(x)$ be any monic polynomial of degree $(n + 1)$ as above, and let

$q_{n+1}(x)$ be the monic orthogonal polynomial as before. Then $r(x) \equiv (W(x) - q_{n+1}(x)) \in \mathcal{P}_n$, so $\langle r, q_{n+1}\rangle = 0$. Now we have

$$\|W\|^2 = \int_a^b (W(x))^2 w(x)\, dx = \int_a^b (q_{n+1}(x) + r(x))^2 w(x)\, dx$$

$$= \int_a^b (q_{n+1}(x))^2 w(x)\, dx + 2\int_a^b q_{n+1}(x) r(x) w(x)\, dx + \int_a^b (r(x))^2 w(x)\, dx$$

$$= \|q_{n+1}\|^2 + 2\langle q_{n+1}, r\rangle + \|r\|^2 = \|q_{n+1}\|^2 + \|r\|^2.$$

Therefore $\|q_{n+1}\| \le \|W\|$ for all such $W(x)$; and so the error bound, (6.41b), is minimized for $W(x) = q_{n+1}(x)$, that is to say, for interpolation at the zeros of the orthogonal polynomial. In the special case in which $[a, b] = [-1, 1]$ and $w(x) = 1$, the minimum bound is achieved by interpolating at the zeros of the $(n + 1)$st-degree Legendre polynomial.

Another indication of the power of interpolating at the zeros of orthogonal polynomials is provided by the following theorem, which guarantees least-squares convergence of the interpolating polynomials.

Theorem 6.8 Erdös-Turán

Let $P_n(x) \in \mathcal{P}_n$ interpolate $f(x)$ at the zeros of $p_{n+1}(x)$ (as in Theorem 6.7). Then

$$\|f - P_n\| \equiv \left(\int_a^b (f(x) - P_n(x))^2 w(x)\, dx\right)^{1/2} \to 0, \qquad \text{as } n \to \infty.$$

Proof. Again for each n, let $p_n^*(x) \in \mathcal{P}_n$ be the best uniform approximation to $f(x)$; and let

$$E_n(f) \equiv \max_{a \le x \le b} |f(x) - p_n^*(x)| \equiv \|f - p_n^*\|_\infty.$$

Then by the triangle inequality, $\|f - P_n\| \le \|f - p_n^*\| + \|p_n^* - P_n\|$. Now

$$\|f - p_n^*\|^2 = \int_a^b (f(x) - p_n^*(x))^2 w(x)\, dx \le (E_n(f))^2 \int_a^b w(x)\, dx.$$

Also since $(p_n^*(x) - P_n(x))^2 \in \mathcal{P}_{2n}$ and the nth Gaussian quadrature is exact in $\mathcal{P}_{2n+1}$ and has positive weights with $\int_a^b w(x)\, dx = \sum_{j=0}^n A_j$, we see that

$$\|p_n^* - P_n\|^2 \equiv \int_a^b (p_n^*(x) - P_n(x))^2 w(x)\, dx$$

$$= \sum_{j=0}^n A_j(p_n^*(x_j) - P_n(x_j))^2 = \sum_{j=0}^n A_j(p_n^*(x_j) - f(x_j))^2$$

$$\le (E_n(f))^2 \sum_{j=0}^n A_j = (E_n(f))^2 \int_a^b w(x)\, dx.$$

Since $\int_a^b w(x)\,dx$ is a constant and $E_n(f) \to 0$ as $n \to \infty$, then both $\|f - p_n^*\|$ and $\|p_n^* - P_n\| \to 0$ as $n \to \infty$. ■

Gaussian quadratures are particularly effective in approximating Fourier coefficients, $\langle f, p_k \rangle \equiv \int_a^b f(x)p_k(x)w(x)\,dx$, but provide the following result, which may be somewhat surprising at first reading. Let $f(x)$ be approximated by the truncated Fourier expansion $f(x) \approx F_n(x) \equiv \Sigma_{k=0}^n \langle f, p_k \rangle p_k(x)$. Using the Gaussian quadrature to approximate $\langle f, p_k \rangle$, we get $\langle f, p_k \rangle \approx \alpha_k \equiv \Sigma_{j=0}^n A_j f(x_j)p_k(x_j)$. Then $F_n(x) \approx \Sigma_{k=0}^n \alpha_k p_k(x)$, but we notice this expression is precisely the interpolating polynomial, $P_n(x)$, as in Theorem 6.7.

6.5.2. Interpolation Using Chebyshev Polynomials

In this section, we will consider some of the practical aspects of interpolation at the zeros of $T_{n+1}(x)$. We have already seen from (5.36) that there are advantages in using these interpolation points. The example given below establishes a useful discrete orthogonality property determined by the zeros of $T_{n+1}(x)$. This relation [and a companion result given in (6.43)] can be used in a variety of ways.

EXAMPLE 6.11. Let $\langle f, g \rangle = \int_{-1}^1 f(x)g(x)(1 - x^2)^{-1/2}\,dx$ and $x_j = \cos[(2j + 1)\pi/2(n + 1)]$, $0 \le j \le n$. For this inner product, the orthonormal polynomials are $p_0(x) = 1/\sqrt{\pi}$ and $p_k(x) = \sqrt{2/\pi}T_k(x)$ for $k \ge 1$ (see Example 5.15b, Chapter 5). By Example 6.9, $A_j = \pi/(n + 1)$, $0 \le j \le n$. Thus by Theorem 6.6, the following relationship holds for $k + m \le 2n$:

$$\frac{2}{n+1} \sum_{j=0}^{n} T_k(x_j)T_m(x_j) = \begin{cases} 0, & k \ne m \\ 1, & k = m > 0 \\ 2, & k = m = 0. \end{cases} \tag{6.42}$$

Formula (6.42) very closely resembles another discrete orthogonality relation for the Chebyshev polynomials (displayed in Example 5.15c), which we can express for $k + m \le 2n$ as

$$\frac{2}{n} \sum_{j=0}^{n}{}'' \; T_k(t_j)T_m(t_j) = \begin{cases} 0, \; k \ne m \\ 1, \; k = m, & 1 \le k \le n-1 \\ 2, \; k = m, & k = 0 \quad \text{or} \quad k = n. \end{cases} \tag{6.43}$$

In (6.43), the points t_j are given by $t_j = \cos[j\pi/n]$, $0 \le j \le n$; and the double prime denotes halving the first and the last terms. Since the validity of (6.42) rests upon the fact that (6.39) is a Gaussian quadrature for $I(f) = \int_{-1}^1 f(x)(1 - x^2)^{-1/2}\,dx$, the similarity of (6.42) and (6.43) leads us to suspect that (6.43) also represents a quadrature for $I(f) = \int_{-1}^1 f(x)(1 - x^2)^{-1/2}\,dx$ of the form

$$Q_n'(f) = \frac{\pi}{n} \sum_{j=0}^{n}{}'' \; f(t_j). \tag{6.44}$$

In investigating the quadrature $Q_n'(f)$, we note first that $I(1) = Q_n'(1) = \pi$ and $I(T_k) = Q_n'(T_k) = 0$ for $1 \le k \le 2n - 1$. However, $I(T_{2n}) = 0$ but $Q_n'(T_{2n}) = \pi$, and so the precision of this quadrature is $(2n - 1)$. To verify these results, we note that $I(T_k) = \langle 1, T_k \rangle = 0$ for $k \ge 1$. To determine $Q_n'(T_k)$, we first suppose $1 \le k \le n$ and use (6.43) with $m = 0$ to find $Q_n'(T_k) = 0$. For $n < k \le 2n$, we let $k = n + m$ and observe that $T_k(t_j) = T_n(t_j)T_m(t_j)$. Thus, using (6.43), we see that $Q_n'(T_k) = 0$ for $n < k < 2n$ and that $Q_n'(T_{2n}) = \pi$. We note that $Q_n'(f)$ is not Gaussian since its precision is $(2n - 1)$ instead of $(2n + 1)$; but it is a powerful formula as we can see from the remarks following (6.40b). The nodes t_j are often called the "practical" Chebyshev nodes. Also observe that if we make the transformation $x = \cos\theta$, then $I(f) = \int_0^\pi f(\cos\theta)\,d\theta$. From (6.44), we see that $Q_n'(f)$ is the composite trapezoidal rule for appoximating $\int_0^\pi f(\cos\theta)\,d\theta$.

From Theorem 6.7 and formula (6.39) we easily find that the polynomial of degree n or less that interpolates $f(x)$ at $x_j = \cos[(2j + 1)\pi/2(n + 1)]$, $0 \le j \le n$, is given by

$$P(x) = \beta_0/2 + \sum_{k=1}^{n} \beta_k T_k(x), \qquad \beta_k = \frac{2}{n+1} \sum_{j=0}^{n} T_k(x_j)f(x_j). \tag{6.45a}$$

A similar formula can be developed for interpolation at the points $t_j = \cos(j\pi/n)$. However since (6.44) is not a Gaussian formula, we cannot directly apply Theorem 6.7. However, we can use (6.43) and mimic the proof of Theorem 6.7 to show that the polynomial of degree n or less that interpolates $f(x)$ at $t_j = \cos(j\pi/n)$, $0 \le j \le$, is (see Problem 8)

$$\tilde{P}(x) = \sum_{k=0}^{n}{}'' \gamma_k T_k(x) \qquad \text{where} \qquad \gamma_k = \frac{2}{n} \sum_{j=0}^{n}{}'' T_k(t_j)f(t_j). \tag{6.45b}$$

We pause to mention that the interpolating polynomials constructed via (6.45a) and (6.45b) can be easily evaluated at a point $x = \alpha$ since they have the form $p(x) = \sum_{k=0}^{n} b_k r_k(x)$ where $\{b_k\}_{k=0}^{n}$ are known constants and each $r_k(x)$ is a constant multiple of $p_k(x)$. We leave to the reader to verify that the efficient algorithm of formula (5.66) can be modified to accomplish this task with $(2n - 1)$ multiplications, once the three-term recursion is known for the $r_k(x)$'s. For example (see Problem 9), if $r_k(x) = T_k(x)$, then we have $T_0(x) = 1$, $T_1(x) = x$, and $T_k(x) = 2xT_{k-1}(x) - T_{k-2}(x)$ for $k \ge 2$. The modification of (5.66) yields in this case

$$\sum_{k=0}^{n} b_k T_k(\alpha) = s_0(\alpha) - \alpha s_1(\alpha) \tag{6.45c}$$

where $s_k(\alpha)$ is defined by $s_{n+1}(\alpha) = s_{n+2}(\alpha) = 0$; and for $k = n, n - 1, \ldots, 0$, by

$$s_k(\alpha) - 2\alpha s_{k+1}(\alpha) + s_{k+2}(\alpha) = b_k.$$

[Note in this particular example that since the coefficient of $s_{k+2}(\alpha)$ equals 1, only $(n + 1)$ multiplications are required.]

We turn now to the infinite Chebyshev expansion for $f(x)$. Recall that

$p_0(x) = 1/\sqrt{\pi}T_0(x)$ and $p_k(x) = \sqrt{2/\pi}T_k(x)$ for $k \geq 1$; so $\langle f, p_0\rangle = 1/\sqrt{\pi}\langle f, T_0\rangle$ and $\langle f, p_k\rangle = \sqrt{2/\pi}\langle f, T_k\rangle$, $k \geq 1$. Thus the Fourier-Chebyshev expansion for $f(x)$ for $-1 \leq x \leq 1$ is

$$f(x) \sim \langle f, p_0\rangle p_0(x) + \sum_{k=1}^{\infty} \langle f, p_k\rangle p_k(x). \tag{6.46a}$$

Often, for the sake of convenience, the normalizing constants of the $p_k(x)$'s are multiplied together and (6.46a) is written in the equivalent form

$$f(x) \sim \sum_{k=0}^{\infty}{}' a_k T_k(x), \qquad a_k = \frac{2}{\pi}\int_{-1}^{1} f(x)T_k(x)(1 - x^2)^{-1/2}\, dx \tag{6.46b}$$

where the prime denotes that the first term is halved.

Using the Gauss-Chebyshev quadrature (6.39) to approximate a_k for $0 \leq k \leq n$, we obtain the interpolating polynomial $P(x)$ of formula (6.45a) as an approximation for $f(x)$ where each $\beta_k = (2/(n + 1)) \sum_{j=0}^{n} T_k(x_j)f(x_j)$ is our approximation to a_k. An alternate approach is to use $\tilde{P}(x)$ of formula (6.45b) as our approximation to $f(x)$ where $\gamma_k = (2/n) \sum_{j=0}^{\prime\prime\, n} T_k(t_j)f(t_j)$ is our approximation to a_k, $0 \leq k \leq n$.

To assess further the accuracy of these interpolations, let us assume that the expansion (6.46b) is absolutely and uniformly convergent to $f(x)$ (which is the case, for example, if $f \in C^2[-1, 1]$). We first consider $\tilde{P}(x)$ in (6.45b); and for a fixed value of m, $0 \leq m \leq n$, we consider the approximation of γ_m for a_m. We can easily verify by trigonometric identities that if $k = 2rn + \alpha$, $r = 0, 1, 2, \ldots, |\alpha| \equiv \beta \leq n$; then $T_k(t_j) = T_\beta(t_j)$, $0 \leq j \leq n$. Making use of (6.43), we obtain for any m

$$\begin{aligned}\gamma_m &= \frac{2}{n} \sum_{j=0}^{n}{}'' \left(\sum_{k=0}^{\infty}{}' a_k T_k(t_j)\right) T_m(t_j) \\ &= \sum_{k=0}^{\infty}{}' a_k \left(\frac{2}{n} \sum_{j=0}^{n}{}'' T_k(t_j)T_m(t_j)\right) \\ &= a_m + (a_{2n-m} + a_{2n+m}) + (a_{4n-m} + a_{4n+m}) + \cdots,\end{aligned} \tag{6.47a}$$

and the resulting approximation of (6.45b)

$$f(x) \approx \sum_{m=0}^{n}{}'' \gamma_m T_m(x). \tag{6.47b}$$

Similarly if we write $k = 2r(n + 1) + \alpha$, we can easily establish the identity $T_\alpha(x_j) = (-1)^r T_{2r(n+1)\pm\alpha}(x_j)$, $0 \leq j \leq n$. Using this and (6.42) in the same manner as above, we obtain for any m

$$\beta_m = a_m - (a_{2n+2-m} + a_{2n+2+m}) + (a_{4n+4-m} + a_{4n+4+m}) - \cdots, \tag{6.48a}$$

which yields the approximation

$$f(x) \approx \sum_{m=0}^{n}{}' \beta_m T_m(x). \tag{6.48b}$$

We leave (Problem 10) for the reader to verify that $|f(x) - \Sigma''^{n}_{m=0} \gamma_m T_m(x)|$ and $|f(x) - \Sigma'^{n}_{m=0} \beta_m T_m(x)|$ are both bounded by $2\ \Sigma^{\infty}_{m=n+1} |a_m|$. Thus, by Section 5.3.2, the error of (6.47b) and (6.48b) can never exceed twice the error of the truncated series, $|f(x) - \Sigma'^{n}_{m=0} a_m T_m(x)|$. We thus note that if the magnitudes of the Fourier coefficients are rapidly decreasing, then both (6.47b) and (6.48b) are good approximations. We also note from (6.47a) and (6.48a) that both γ_m and β_m are most likely to agree closely with a_m when m is small. We expect the most discrepancy in (6.47a) when $m = n - 1$ and in (6.48a) when $m = n$; in those cases we see that $\gamma_{n-1} \approx a_{n-1} + a_{n+1}$ and $\beta_n \approx a_n - a_{n+2}$, respectively. However if n is sufficiently large, then the coefficients a_{n-1}, a_{n+1}, and a_{n+2} should be relatively small and should not significantly affect the accuracy.

6.5.3. Clenshaw-Curtis Quadrature

We note that any time we have an approximation for $f(x)$ of the form $f(x) \approx p(x) \equiv \Sigma^{n}_{k=0} b_k T_k(x)$, then we can easily construct a numerical integration formula from the approximation. This fact follows from the simple observation that indefinite integration of $T_k(x)$ yields

$$\begin{aligned}\int T_k(x)\,dx &= -\int \cos(k\theta)\sin(\theta)\,d\theta \\ &= -\frac{1}{2}\int (\sin[(k+1)\theta] - \sin[(k-1)\theta])\,d\theta \qquad (6.49a)\\ &= \frac{1}{2}\left(\frac{T_{k+1}(x)}{k+1} - \frac{T_{k-1}(x)}{k-1}\right), \qquad k \geq 2,\end{aligned}$$

and

$$\int T_0(x)\,dx = T_1(x), \qquad \int T_1(x)\,dx = \frac{1}{4}(T_0(x) + T_2(x)). \qquad (6.49b)$$

Given $p(x)$ as above, then the result of the indefinite integration of $p(t)$ is an expression of the form

$$\int_{-1}^{x} p(t)\,dt = \sum_{k=0}^{n} b_k \int_{-1}^{x} T_k(t)\,dt \equiv \sum_{k=0}^{n+1} A_k T_k(x) \equiv P(x). \qquad (6.50)$$

Using the integral formulas (6.49a) and (6.49b) and equating like coefficients of each $T_k(x)$, we have the following equations for each A_k:

$$A_{n+1} = \frac{b_n}{2(n+1)}, \qquad A_n = \frac{b_{n-1}}{2n}, \qquad A_1 = b_0 - \frac{b_2}{2}, \qquad (6.51a)$$

and

$$A_k = \frac{1}{2k}(b_{k-1} - b_{k+1}), \qquad \text{for } 2 \leq k \leq n-1.$$