(see [16]) ensures that for each $f \in C[a,b]$ there exists a sequence of polynomials $p_n \in P_n$ such that $\|p_n - f\|_\infty \to 0$ as $n \to \infty$. As a consequence of the Chebyshev alternation theorem from approximation theory (see [16]), for the uniquely determined best approximation $\tilde{p}_n$ to f in the maximum norm with respect to P_n, the error $\tilde{p}_n - f$ has at least $n+1$ zeros in $[a,b]$. Then taking the sequence of these zeros as the sequence of interpolation points implies the statement of the theorem. □

Theorem 8.17 (Faber) *For each sequence of interpolation points* $(x_j^{(n)})$ *there exists a function* $f \in C[a,b]$ *such that the sequence* $(L_n f)$ *of interpolation polynomials* $L_n f \in P_n$ *does not converge to* f *uniformly on* $[a,b]$.

Proof. This is a consequence of the uniform boundedness principle, Theorem 12.7. It implies that from the convergence of the sequence $(L_n f)$ for all $f \in C[a,b]$ it follows that there must exist a constant $C > 0$ such that $\|L_n\|_\infty \le C$ for all $n \in \mathbb{N}$. Then the statement of the theorem is obtained by showing that the interpolation operator L_n satisfies $\|L_n\|_\infty \ge c \ln n$ for all $n \in \mathbb{N}$ and some $c > 0$ (see [16]). □

We conclude this section by briefly describing Hermite interpolation, where in addition to the values of the polynomial, the values of its first derivative at the interpolation points are also prescribed.

Theorem 8.18 *Given* $n+1$ *distinct points* $x_0, \dots, x_n \in [a,b]$ *and* $2n+2$ *values* $y_0, \dots, y_n \in \mathbb{R}$ *and* $y'_0, \dots, y'_n \in \mathbb{R}$, *there exists a unique polynomial* $p_{2n+1} \in P_{2n+1}$ *with the property*

$$p_{2n+1}(x_j) = y_j, \quad p'_{2n+1}(x_j) = y'_j, \quad j = 0, \dots, n. \tag{8.10}$$

This Hermite interpolation polynomial *is given by*

$$p_{2n+1} = \sum_{k=0}^{n} [y_k H_k^0 + y'_k H_k^1] \tag{8.11}$$

with the Hermite factors

$$H_k^0(x) := [1 - 2\ell'_k(x_k)(x - x_k)]\,[\ell_k(x)]^2, \quad H_k^1(x) := (x - x_k)\,[\ell_k(x)]^2$$

expressed in terms of the Lagrange factors from Theorem 8.3.

Proof. Obviously, the polynomial p_{2n+1} belongs to P_{2n+1}, since the Hermite factors have degree $2n+1$. From (8.3), by elementary calculations it can be seen that (see Problem 8.7)

$$\begin{aligned} H_k^0(x_j) &= H_k^{1\prime}(x_j) = \delta_{jk}, \\ H_k^{0\prime}(x_j) &= H_k^1(x_j) = 0, \end{aligned} \qquad j,k = 0,\dots,n. \tag{8.12}$$

From this it follows that the polynomial (8.11) satisfies the Hermite interpolation property (8.10).

To prove uniqueness of the Hermite interpolation polynomial we assume that $p_{2n+1,1}, p_{2n+1,2} \in P_{2n+1}$ are two polynomials having the interpolation property (8.10). Then the difference $p_{2n+1} := p_{2n+1,1} - p_{2n+1,2}$ satisfies

$$p_{2n+1}(x_j) = p'_{2n+1}(x_j) = 0, \quad j = 0, \ldots, n;$$

i.e., the polynomial $p_{2n+1} \in P_{2n+1}$ has $n+1$ zeros of order two and therefore, by Theorem 8.1, must be identically equal to zero. This implies that $p_{2n+1,1} = p_{2n+1,2}$. □

The main application of Hermite interpolation consists in the approximation of a given function $f \in C^1[a,b]$ by interpolating its function values and the values of its derivative at $n+1$ distinct points $x_0, \ldots, x_n \in [a,b]$. By

$$H_n : C^1[a,b] \to P_{2n+1}$$

we denote the *Hermite interpolation operator* that maps continuously differentiable functions $f : [a,b] \to \mathbb{R}$ into the uniquely determined Hermite interpolation polynomial $H_n f \in P_{2n+1}$ with the property

$$(H_n f)(x_j) = f(x_j), \quad (H_n f)'(x_j) = f'(x_j), \quad j = 0, \ldots, n.$$

The following theorem can be proven analogously to Theorem 8.10 (see Problem 8.8).

Theorem 8.19 *Let $f : [a,b] \to \mathbb{R}$ be $(2n+2)$-times continuously differentiable. Then the remainder $R_n f := f - H_n f$ for Hermite interpolation with $n+1$ distinct points $x_0, \ldots, x_n \in [a,b]$ can be represented in the form*

$$(R_n f)(x) = \frac{f^{(2n+2)}(\xi)}{(2n+2)!} \prod_{j=0}^{n} (x - x_j)^2, \quad x \in [a,b], \tag{8.13}$$

for some $\xi \in [a,b]$ depending on x.

8.2 Trigonometric Interpolation

In applications, quite frequently there occur periodic functions, i.e., functions with the property

$$f(t+T) = f(t), \quad t \in \mathbb{R},$$

for some $T > 0$. For example, functions defined on closed planar or spatial curves always may be viewed as periodic functions. Polynomial interpolation is not appropriate for periodic functions, since algebraic polynomials

Theorem 9.18 *The weights of the Gaussian quadrature formulae are all positive.*

Proof. Define

$$f_k(x) := \left[\frac{q_{n+1}(x)}{x - x_k}\right]^2, \quad k = 0, \ldots, n.$$

Then

$$a_k[q'_{n+1}(x_k)]^2 = \sum_{j=0}^{n} a_j f_k(x_j) = \int_a^b w(x) f_k(x)\, dx > 0,$$

since $f_k \in P_{2n}$, and the theorem is proven. □

Corollary 9.19 *The sequence of Gaussian quadrature formulae is convergent.*

Proof. For each polynomial p we have

$$Q_n(p) = \int_a^b w(x) p(x)\, dx,$$

provided that $2n + 1$ is greater than or equal to the degree of p. From their proofs it is obvious that Theorem 9.10 and its Corollary 9.11 remain valid for the integral with the weight function w. Hence, the statement of the theorem follows from Theorem 9.18. □

Theorem 9.20 *Let $f \in C^{2n+2}[a, b]$. Then the error for the Gaussian quadrature formula of order n is given by*

$$\int_a^b w(x) f(x)\, dx - \sum_{k=0}^{n} a_k f(x_k) = \frac{f^{(2n+2)}(\xi)}{(2n+2)!} \int_a^b w(x)[q_{n+1}(x)]^2 dx$$

for some $\xi \in [a, b]$.

Proof. Recall the Hermite interpolation polynomial $H_n f \in P_{2n+1}$ for f from Theorem 8.18. Since $(H_n f)(x_k) = f(x_k)$, $k = 0, \ldots, n$, for the error

$$E_n(f) := \int_a^b w(x) f(x)\, dx - \sum_{k=0}^{n} a_k f(x_k)$$

we can write

$$E_n(f) = \int_a^b w(x)[f(x) - (H_n f)(x)]\, dx.$$

Then as in the proofs of Theorems 9.7 and 9.8, using the mean value theorem we obtain

$$E_n(f) = \frac{f(z) - (H_n f)(z)}{[q_{n+1}(z)]^2} \int_a^b w(x)[q_{n+1}(x)]^2 dx$$

for some $z \in [a, b]$. Now the proof is finished with the aid of the error representation for Hermite interpolation from Theorem 8.19. □

The first Bernoulli polynomials are given by

$$B_0(x) = 1, \quad B_1(x) = x - \frac{1}{2}, \quad B_2(x) = \frac{1}{2}x^2 - \frac{1}{2}x + \frac{1}{12}$$

We note that the normalization (9.22) is equivalent to

$$B_n(0) = B_n(1), \quad n = 2, 3, \ldots. \tag{9.23}$$

Lemma 9.24 *The Bernoulli polynomials have the symmetry property*

$$B_n(x) = (-1)^n B_n(1-x), \quad x \in \mathbb{R}, \quad n = 0, 1, \ldots. \tag{9.24}$$

Proof. Obviously (9.24) holds for $n = 0$. Assume that (9.24) has been proven for some $n \geq 0$. Then, integrating (9.24), we obtain

$$B_{n+1}(x) = (-1)^{n+1} B_{n+1}(1-x) + \beta_{n+1}$$

for some constant β_{n+1}. The condition (9.22) implies that $\beta_{n+1} = 0$, and therefore (9.24) is also valid for $n+1$. □

Lemma 9.25 *The Bernoulli polynomials B_{2m+1}, $m = 1, 2, \ldots$, of odd degree have exactly three zeros in $[0,1]$, and these zeros are at the points 0, $1/2$, and 1. The Bernoulli polynomials B_{2m}, $m = 0, 1, \ldots$, of even degree satisfy $B_{2m}(0) \neq 0$.*

Proof. From (9.23) and (9.24) we conclude that B_{2m+1} vanishes at the points 0, 1/2, and 1. We prove by induction that these are the only zeros of B_{2m+1} in $[0,1]$. This is true for $m = 1$, since B_3 is a polynomial of degree three. Assume that we have proven that B_{2m+1} has only the three zeros 0, 1/2, and 1 in $[0,1]$, and assume that B_{2m+3} has an additional zero α in $[0,1]$. Because of the symmetry (9.24) we may assume that $\alpha \in (0, 1/2)$. Then, by Rolle's theorem, we conclude that B_{2m+2} has at least one zero in $(0, \alpha)$ and also at least one zero in $(\alpha, 1/2)$. Again by Rolle's theorem this implies that B_{2m+1} has a zero in $(0, 1/2)$, which contradicts the induction assumption.

From the zeros of B_{2m+1}, by Rolle's theorem it follows that B_{2m} has a zero in $(0, 1/2)$. Assume that $B_{2m}(0) = 0$. Then, by Rolle's theorem, B_{2m-1} has a zero in $(0, 1/2)$, which contradicts the first part of the lemma. □

By $\tilde{B}_n : \mathbb{R} \to \mathbb{R}$ we denote the periodic extension of the Bernoulli polynomial B_n; i.e., $\tilde{B}_n$ has period 1 and $\tilde{B}_n(x) = B_n(x)$ for $0 \leq x \leq 1$. The Fourier series of the periodic functions $\tilde{B}_n$ are given by

$$\tilde{B}_{2m}(x) = 2(-1)^{m-1} \sum_{k=1}^{\infty} \frac{\cos 2\pi k x}{(2\pi k)^{2m}} \tag{9.25}$$

and

$$\tilde{B}_{2m-1}(x) = 2(-1)^{m} \sum_{k=1}^{\infty} \frac{\sin 2\pi k x}{(2\pi k)^{2m-1}} \tag{9.26}$$

for $m = 1, 2, \ldots$. This follows from (9.21) and (9.22) and the elementary Fourier expansion for the piecewise linear function $\tilde{B}_1$ (see Problem 9.13).

Let $x_k = a + kh$, $k = 0, \ldots, n$, be an equidistant subdivision of the interval $[a, b]$ with step size $h = (b - a)/n$ and recall the definition of the trapezoidal sum

$$T_h(f) := h \left[\frac{1}{2} f(x_0) + f(x_1) + \cdots + f(x_{n-1}) + \frac{1}{2} f(x_n) \right]$$

for $f \in C[a, b]$.

Theorem 9.26 *Let $f : [a, b] \to \mathbb{R}$ be m times continuously differentiable for $m \geq 2$. Then we have the* Euler–Maclaurin expansion

$$\int_a^b f(x)\, dx = T_h(f) - \sum_{j=1}^{\left[\frac{m}{2}\right]} \frac{b_{2j} h^{2j}}{(2j)!} \left[f^{(2j-1)}(b) - f^{(2j-1)}(a) \right]$$
$$+ (-1)^m h^m \int_a^b \tilde{B}_m \left(\frac{x - a}{h} \right) f^{(m)}(x)\, dx, \tag{9.27}$$

where $\left[\frac{m}{2}\right]$ denotes the largest integer smaller than or equal to $\frac{m}{2}$.

Proof. Let $g \in C^m[0, 1]$. Then, by $m - 1$ partial integrations and using (9.23) we find that

$$\int_0^1 B_1(z) g'(z)\, dz = \sum_{j=2}^{m} (-1)^j B_j(0) [g^{(j-1)}(1) - g^{(j-1)}(0)]$$
$$- (-1)^m \int_0^1 B_m(z) g^{(m)}(z)\, dz.$$

Combining this with the partial integration

$$\int_0^1 B_1(z) g'(z)\, dz = \frac{1}{2} [g(1) + g(0)] - \int_0^1 g(z)\, dz$$

and observing that the odd Bernoulli numbers vanish leads to

$$\int_0^1 g(z)\, dz = \frac{1}{2} [g(0) + g(1)] - \sum_{j=1}^{\left[\frac{m}{2}\right]} \frac{b_{2j}}{(2j)!} [g^{(2j-1)}(1) - g^{(2j-1)}(0)]$$
$$+ (-1)^m \int_0^1 B_m(z) g^{(m)}(z)\, dz.$$

Now we substitute $x = x_k + hz$ and $g(z) = f(x_k + hz)$ to obtain

$$\int_{x_k}^{x_{k+1}} f(x)\,dx = \frac{h}{2}\,[f(x_k) + f(x_{k+1})]$$

$$-\sum_{j=1}^{[\frac{m}{2}]} \frac{b_{2j}h^{2j}}{(2j)!}\,[f^{(2j-1)}(x_{k+1}) - f^{(2j-1)}(x_k)]$$

$$+(-1)^m h^m \int_{x_k}^{x_{k+1}} B_m\left(\frac{x-a}{h}\right) f^{(m)}(x)\,dx.$$

Finally, we sum the last equation for $k = 0, \dots, n-1$ to arrive at the Euler–Maclaurin expansion (9.27). □

For 2π-periodic continuous functions $f : \mathbb{R} \to \mathbb{R}$ the trapezoidal rule coincides with the *rectangular rule*

$$\int_0^{2\pi} f(x)\,dx \approx \frac{2\pi}{n} \sum_{k=1}^{n} f\left(\frac{2\pi k}{n}\right)$$

For its error

$$E_n(f) := \int_0^{2\pi} f(x)\,dx - \frac{2\pi}{n} \sum_{k=1}^{n} f\left(\frac{2\pi k}{n}\right)$$

we have the following corollary of the Euler–Maclaurin expansion.

Corollary 9.27 *Let $f : \mathbb{R} \to \mathbb{R}$ be $(2m+1)$-times continuously differentiable and 2π-periodic for $m \in \mathbb{N}$ and let $n \in \mathbb{N}$. Then for the error of the rectangular rule we have*

$$|E_n(f)| \le \frac{C}{n^{2m+1}} \int_0^{2\pi} |f^{(2m+1)}(x)|\,dx,$$

where

$$C := 2\sum_{k=1}^{\infty} \frac{1}{k^{2m+1}}\ .$$

Proof. From Theorem 9.26 we have that

$$E_n(f) = -\left(\frac{2\pi}{n}\right)^{2m+1} \int_0^{2\pi} \tilde{B}_{2m+1}\left(\frac{2\pi x}{n}\right) f^{(2m+1)}(x)\,dx,$$

and the estimate follows from the inequality

$$|\tilde{B}_{2m+1}(x)| \le 2\sum_{k=1}^{\infty} \frac{1}{(2\pi k)^{2m+1}}\ , \quad x \in \mathbb{R},$$

which is a consequence of (9.26). □

Corollary 9.27 illustrates why for periodic functions the simple rectangular rule is superior to any other quadrature rule (see Problem 9.12). Note that the rectangular rule can also be obtained by integrating the trigonometric interpolation polynomials of Theorems 8.24 and 8.25.

In the following theorem we give an example of derivative-free error estimates for numerical quadrature rules in the spirit of Davis [15]. They have the advantage that they do not need the computation of higher derivatives for the evaluation of the estimates. However, they require the integrand to be analytic, and their proofs need complex analysis.

Theorem 9.28 *Let $f : \mathbb{R} \to \mathbb{R}$ be analytic and 2π-periodic. Then there exists a strip $D = \mathbb{R} \times (-a, a) \subset \mathbb{C}$ with $a > 0$ such that f can be extended to a holomorphic and 2π-periodic bounded function $f : D \to \mathbb{C}$. The error for the rectangular rule can be estimated by*

$$|E_n(f)| \le \frac{4\pi M}{e^{na} - 1},$$

where M denotes a bound for the holomorphic function f on D.

Proof. Since $f : \mathbb{R} \to \mathbb{R}$ is analytic, at each point $x \in \mathbb{R}$ the Taylor expansion provides a holomorphic extension of f into some open disk in the complex plane with radius $r(x) > 0$ and center x. The extended function again has period 2π, since the coefficients of the Taylor series at x and at $x + 2\pi$ coincide for the 2π–periodic function $f : \mathbb{R} \to \mathbb{R}$. The disks corresponding to all points of the interval $[0, 2\pi]$ provide an open covering of $[0, 2\pi]$. Since $[0, 2\pi]$ is compact, a finite number of these disks suffices to cover $[0, 2\pi]$. Then we have an extension into a strip D with finite width $2a$ contained in the union of the finite number of disks. Without loss of generality we may assume that f is bounded on D.

From the residue theorem we have that

$$\int_{i\alpha}^{i\alpha+2\pi} \cot\frac{nz}{2}\, f(z)\, dz - \int_{-i\alpha}^{-i\alpha+2\pi} \cot\frac{nz}{2}\, f(z)\, dz = -\frac{4\pi i}{n} \sum_{k=1}^{n} f\left(\frac{2\pi k}{n}\right)$$

for each $0 < \alpha < a$. This implies that

$$\mathrm{Re} \int_{i\alpha}^{i\alpha+2\pi} i\cot\frac{nz}{2}\, f(z)\, dz = \frac{2\pi}{n} \sum_{k=1}^{n} f\left(\frac{2\pi k}{n}\right),$$

since by the Schwarz reflection principle, f enjoys the symmetry property $f(\bar{z}) = \overline{f(z)}$. By Cauchy's integral theorem we have

$$\mathrm{Re} \int_{i\alpha}^{i\alpha+2\pi} f(z)\, dz = \int_0^{2\pi} f(x)\, dx,$$

and combining the last two equations yields

$$E_n(f) = \mathrm{Re} \int_{i\alpha}^{i\alpha+2\pi} \left(1 - i\cot\frac{nz}{2}\right) f(z)\, dz$$

for all $0 < \alpha < a$. Now the estimate follows from

$$\left|1 - i\cot\frac{nz}{2}\right| \le \frac{2}{e^{n\alpha} - 1}$$

for $\operatorname{Im} z = \alpha$ and then passing to the limit $\alpha \to a$. □

The estimate shows that for periodic analytic functions the rectangular rule is of exponential order; i.e., doubling the number of quadrature points doubles the number of correct digits in the approximate value for the integral.

9.5 Romberg Integration

We now proceed with describing the *extrapolation method* due to Richardson (1927). Its basic idea is to derive high-order approximation methods from simple low-order methods. It can be applied to a variety of formulae in numerical analysis, and its application to the Euler–Maclaurin expansion was suggested by Romberg in 1955.

Recall the composite trapezoidal rule

$$T_h^1(f) := h\left[\frac{1}{2}\,f(a) + \sum_{k=1}^{n-1} f(a+kh) + \frac{1}{2}\,f(b)\right]$$

with step size $h = (b-a)/n$. If f is four-times continuously differentiable, by the Euler–Maclaurin expansion from Theorem 9.26 we have an error representation of the form

$$\int_a^b f(x)\,dx = T_h^1(f) + \gamma_1 h^2 + O(h^4)$$

for some constant γ_1 depending on f but not on h. Hence, for half the step size, we have that

$$\int_a^b f(x)\,dx = T_{\frac{h}{2}}^1(f) + \gamma_1\,\frac{h^2}{4} + O(h^4).$$

From these two equations we can eliminate the terms containing h^2; i.e., we multiply the first equation by $-1/3$ and the second equation by $4/3$ and add both equations to obtain

$$\int_a^b f(x)\,dx = \frac{1}{3}\left[4\,T_{\frac{h}{2}}^1(f) - T_h^1(f)\right] + O(h^4).$$

Hence, the linear combination

$$T_h^2(f) := \frac{1}{3}\left[4\,T_{\frac{h}{2}}^1(f) - T_h^1(f)\right]$$