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FAMILIES OF EULER-MACLAURIN FORMULAE FOR COMPOSITE GAUSS-LEGENDRE AND LOBATTO QUADRATURES

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A b s t r a c t. Beside a short account on the Euler-Maclaurin formula, using a recent progress in variable-precision arithmetic and symbolic computation and the corresponding MATHEMATICA *package* `OrthogonalPolynomials` [*Facta Univ. Ser. Math. Inform.* **19** (2004), 17 − 36; *Math. Balkanica* **26** (2012), 169−184], *we obtain extensions of the Euler-Maclaurin formula for the composite (shifted) Gauss-Legendre formula, as well as for its Lobatto modification. Some special cases are also presented.*

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1. *Introduction*

The Euler-Maclaurin summation formula plays an important role in the broad area of numerical analysis, analytic number theory, and the theory of asymptotic expansions, as well as in many applications in other fields. In connection with the so-called Basel problem (or in modern terminology, with determining $\zeta(2)$), in 1732 Leonhard Euler discovered this formula,

$$\begin{aligned}\sum_{k=0}^{n} f(k) &= \int_0^n f(x)\,\mathrm{d}x + \frac{1}{2}(f(0)+f(n)) \\ &\quad + \sum_{j=1}^{r} \frac{B_{2j}}{(2j)!}\Big[f^{(2j-1)}(n) - f^{(2j-1)}(0)\Big] + E_r(f), \qquad (1.1)\end{aligned}$$

which holds for any $n, r \in \mathbb{N}$ and $f \in C^{2r}[0,n]$, where B_{2j} are Bernoulli numbers ($B_0 = 1$, $B_1 = -1/2$, $B_2 = 1/6$, $B_3 = 0$, $B_4 = -1/30, \ldots$). This formula was also found independently by Maclaurin. While in Euler's case the formula (1.1) was applied for computing slowly converging infinite series, in the second one Maclaurin used it to calculate integrals. A history of this formula was given by Barnes [3], and some details can be found in [19], [1], [11], [12], [5].

Bernoulli numbers B_n, $n = 0, 1, \ldots$, can be expressed as values at zero of the corresponding Bernoulli polynomials, which are defined by the generating function

$$\frac{t\mathrm{e}^{xt}}{\mathrm{e}^t - 1} = \sum_{j=0}^{\infty} \frac{B_j(x)t^j}{j!}.$$

Bernoulli polynomials play a similar role in numerical analysis and approximation theory like orthogonal polynomials. First few polynomials are

$$B_0(x) = 1, \quad B_1(x) = x - \frac{1}{2}, \quad B_2(x) = x^2 - x + \frac{1}{6}, \quad B_3(x) = x^3 - \frac{3x^2}{2} + \frac{x}{2},$$

$$B_4(x) = x^4 - 2x^3 + x^2 - \frac{1}{30}, \quad B_5(x) = x^5 - \frac{5x^4}{2} + \frac{5x^3}{3} - \frac{x}{6}, \quad \text{etc.}$$

Some interesting properties of these polynomials are

$$B_n'(x) = nB_{n-1}(x), \quad B_n(1-x) = (-1)^n B_n(x), \quad \int_0^1 B_n(x)\,\mathrm{d}x = 0 \quad (n \in \mathbb{N}).$$

The error term $E_r(f)$ in (1.1) can be expressed in the form (cf. [5])

$$E_r(f) = (-1)^r \sum_{k=1}^{+\infty} \int_0^n \frac{\mathrm{e}^{\mathrm{i}2\pi kt} + \mathrm{e}^{-\mathrm{i}2\pi kt}}{(2\pi k)^{2r}} f^{(2r)}(x)\,\mathrm{d}x,$$

or in the form

$$E_r(f) = -\int_0^n \frac{B_{2r}(x - \lfloor x \rfloor)}{(2r)!} f^{(2r)}(x)\,\mathrm{d}x, \tag{1.2}$$

where $\lfloor x \rfloor$ denotes the largest integer that is not greater than x. Supposing $f \in C^{2r+1}[0,n]$, after an integration by parts in (1.2) and recalling that the odd Bernoulli numbers are zero, we get (cf. [14, p. 455])

$$E_r(f) = \int_0^n \frac{B_{2r+1}(x - \lfloor x \rfloor)}{(2r+1)!} f^{(2r+1)}(x)\,\mathrm{d}x. \tag{1.3}$$

If $f \in C^{2r+2}[0,n]$, using Darboux's formula one can obtain (1.1), with

$$E_r(f) = \frac{1}{(2r+2)!} \int_0^1 [B_{2r+2} - B_{2r+2}(x)] \left(\sum_{k=0}^{n-1} f^{(2r+2)}(k+x) \right) \mathrm{d}x \tag{1.4}$$

(cf. Whittaker & Watson [26, p. 128]). This expression for $E_r(f)$ can be also derived from (1.3), writting it in the form

$$\begin{aligned} E_r(f) &= \int_0^1 \frac{B_{2r+1}(x)}{(2r+1)!} \left(\sum_{k=0}^{n-1} f^{(2r+1)}(k+x) \right) \mathrm{d}x \\ &= \int_0^1 \frac{B'_{2r+2}(x)}{(2r+2)!} \left(\sum_{k=0}^{n-1} f^{(2r+1)}(k+x) \right) \mathrm{d}x, \end{aligned}$$

and then by an integration by parts, the last expression becomes

$$\left[\frac{B_{2r+2}(x)}{(2r+2)!} \left(\sum_{k=0}^{n-1} f^{(2r+1)}(k+x) \right) \right]_0^1 - \int_0^1 \frac{B_{2r+2}(x)}{(2r+2)!} \left(\sum_{k=0}^{n-1} f^{(2r+2)}(k+x) \right) \mathrm{d}x.$$

Because of $B_{2r+2}(1) = B_{2r+2}(0) = B_{2r+2}$, $E_r(f)$ can be represented in the form (1.4).

Since $(-1)^r\,[B_{2r+2} - B_{2r+2}(x)] \ge 0$ on $[0,1]$ and

$$\int_0^1 [B_{2r+2} - B_{2r+2}(x)]\,\mathrm{d}t = B_{2r+2},$$

according to the *Second Mean Value Theorem for Integrals*, there exists $\eta \in (0,1)$ such that

$$E_r(f) = \frac{B_{2r+2}}{(2r+2)!} \left(\sum_{k=0}^{n-1} f^{(2r+2)}(k+\eta) \right) = n\,\frac{B_{2r+2}}{(2r+2)!} f^{(2r+2)}(\xi), \quad 0 < \xi < n. \tag{1.5}$$

Remark 1.1 The Euler-Maclaurin summation formula is implemented in Mathematica as the function `NSum` with option `Method -> Integrate`.

Practicaly, the Euler-Maclaurin summation formula (1.1) is related with the so-called composite trapezoidal rule,

$$T_n f := \sum_{k=0}^{n}{}'' f(k) = \frac{1}{2}f(0) + \sum_{k=1}^{n-1} f(k) + \frac{1}{2}f(n).$$

Namely,

$$T_n f - I_n f = \sum_{j=1}^{r} \frac{B_{2j}}{(2j)!}\Big[f^{(2j-1)}(n) - f^{(2j-1)}(0)\Big] + E_r^T(f), \tag{1.6}$$

where $I_n f := \int_0^n f(x)\,\mathrm{d}x$ and the remainder term $E_r^T(f)$ is given by (1.5) if the function f belongs to $C^{2r+2}[0,n]$.

Similarly, for a quadrature sum with values of the function f at the points $x = k + \frac{1}{2}$, $k = 0, 1, \ldots, n-1$, i.e., for the midpoint rule

$$M_n f := \sum_{k=0}^{n-1} f\Big(k + \frac{1}{2}\Big),$$

there exists the so-called second Euler-Maclaurin summation formula

$$M_n f - I_n f = \sum_{j=1}^{r} \frac{(2^{1-2j}-1)B_{2j}}{(2j)!}\Big[f^{(2j-1)}(n) - f^{(2j-1)}(0)\Big] + E_r^M(f), \tag{1.7}$$

for which

$$E_r^M(f) = n\,\frac{(2^{-1-2r}-1)B_{2r+2}}{(2r+2)!} f^{(2r+2)}(\xi), \qquad 0 < \xi < n,$$

when $f \in C^{2r+2}[0,n]$ (cf. [20, p. 157]).

The both formulas, (1.6) and (1.7), can be unified as

$$Q_n f - I_n f = \sum_{j=1}^{r} \frac{B_{2j}(\tau)}{(2j)!}\Big[f^{(2j-1)}(n) - f^{(2j-1)}(0)\Big] + E_r^Q(f),$$

where $\tau = 0$ for $Q_n \equiv T_n$ and $\tau = 1/2$ for $Q_n \equiv M_n$. It is true, because of the fact that [24, p. 765] (see also [7])

$$B_j(0) = B_j \quad \text{and} \quad B_j\Big(\frac{1}{2}\Big) = (2^{1-j}-1)B_j.$$

If we take a combination of T_nf and M_nf as $Q_nf = S_nf = \frac{1}{3}(T_nf + 2M_nf)$, which is, in fact, the well-known classical composite Simpson rule,

$$S_nf := \frac{1}{3}\left[\frac{1}{2}f(0) + \sum_{k=1}^{n-1} f(k) + 2\sum_{k=0}^{n-1} f\Big(k+\frac{1}{2}\Big) + \frac{1}{2}f(n)\right],$$

we obtain

$$S_nf - I_nf = \sum_{j=2}^{r} \frac{(4^{1-j}-1)B_{2j}}{3(2j)!}\Big[f^{(2j-1)}(n) - f^{(2j-1)}(0)\Big] + E_r^S(f). \quad (1.8)$$

Notice that the summation on the right hand-side in the previous equality starts with $j = 2$, because the term for $j = 1$ vanishes. For $f \in C^{2r+2}[0, n]$ it can be proved that there exists $\xi \in (0, n)$, such that

$$E_r^S(f) = n\,\frac{(4^{-r}-1)B_{2r+2}}{3(2r+2)!} f^{(2r+2)}(\xi).$$

Some periodic analogues of the Euler-Maclaurin formula with applications to number theory have been developed by Berndt and Schoenfeld [4]. In the last section of [4], they showed how the composite Newton-Cotes quadrature formulas (Simpson's parabolic and Simpson's three-eighths rules), as well as various other quadratures (e.g., Weddle's composite rule), can be derived from special cases of their periodic Euler-Maclaurin formula, including explicit formulas for the remainder term. Also, in the papers [8], [23], [25], the authors considered some generalizations of the Euler-Maclaurin formula for some particular Newton-Cotes rules, as well as for 2- and 3-point Gauss-Legendre and Lobatto formulas (see also [2], [9], [16], [17]).

A recent progress in variable-precision arithmetic and symbolic computation has enabled a development of symbolic/variable-precision software for orthogonal polynomials and quadratures of Gaussian type, as well as for their many generalizations. The corresponding software is available today (Gautschi's package `SOPQ` in MATLAB (cf. [21]) and our MATHEMATICA package `OrthogonalPolynomials` [6], [22]).

Using this advantage in this paper we give extensions of Euler-Maclaurin formulae by replacing Q_n by the composite Gauss-Legendre shifted formula, as well as by its Lobatto modification. Several special cases were obtained by using our MATHEMATICA package `OrthogonalPolynomials`.

2. *Euler-Maclaurin formula based on the composite Gauss-Legendre formula*

Let $w_\nu = w_\nu^G$ and $\tau_\nu = \tau_\nu^G$, $\nu = 1, \ldots, m$, be weights (Christoffel numbers) and nodes of the Gauss-Legendre quadrature formula on $[0, 1]$,

$$\int_0^1 f(x)\,\mathrm{d}x = \sum_{\nu=1}^{m} w_\nu^G f(\tau_\nu^G) + R_m^G(f), \tag{2.1}$$

where the nodes τ_ν are zeros of the shifted (monic) Legendre polynomial

$$\pi_m(x) = \binom{2m}{m}^{-1} P_m(2x-1).$$

Degree of its algebraic precision is $d = 2m - 1$, i.e., $R_m^G(f) = 0$ for all algebraic polynomials of degree $\le 2m - 1$. The quadrature sum in (2.1) we denote by $Q_m^G f$, i.e.,

$$Q_m^G f = \sum_{\nu=1}^{m} w_\nu^G f(\tau_\nu^G).$$

A characterization of the Gaussian quadrature (2.1) can be done via an eigenvalue problem for the symmetric tridiagonal Jacobi matrix (cf. [18, p. 326]),

$$J_m = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & \mathbf{O} \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{m-1}} \\ \mathbf{O} & & & \sqrt{\beta_{m-1}} & \alpha_{m-1} \end{bmatrix}, \tag{2.2}$$

constructed with the three-term recurrence coefficients,

$$\alpha_k = 1/2, \quad \beta_k = \frac{1}{16}\cdot\frac{1}{1-(2k)^{-2}}, \quad k \in \mathbb{N}.$$

The nodes $\tau_\nu = \tau_\nu^G$ are the eigenvalues of J_m and the weights w_ν^G are given by $w_\nu^G = \beta_0 v_{\nu,1}^2$, $\nu = 1, \ldots, m$, where $\beta_0 = \mu_0 = \int_0^1 \mathrm{d}x = 1$ and $v_{\nu,1}$ is the first component of the normalized eigenvector $\mathbf{v}_\nu = [v_{\nu,1} \ \cdots \ v_{\nu,m}]^T$ (with ${\mathbf{v}_\nu}^T \mathbf{v}_\nu = 1$) corresponding to the eigenvalue τ_ν,

$$J_m \mathbf{v}_\nu = \tau_\nu \mathbf{v}_\nu, \quad \nu = 1, \ldots, m.$$

Golub and Welsch [13] gave an efficient procedure for constructing the Gaussian quadrature rules by simplifying the well-known QR algorithm so that only the first components of the eigenvectors are computed. Such a procedure is implemented in several programming packages including the most known `ORTHPOL` given by Gautschi [10], as well as in the previous mentioned packages `SOPQ` (in MATLAB) and `OrthogonalPolynomials` (in MATHEMATICA).

The corresponding composite Gauss-Legendre sum for approximating $I_n f := \int_0^n f(x)\,\mathrm{d}x$ can be expressed in the form

$$G_m^{(n)} f = \sum_{k=0}^{n-1} Q_m^G f(k+\cdot) = \sum_{\nu=1}^{m} w_\nu^G \sum_{k=0}^{n-1} f(k+\tau_\nu^G). \tag{2.3}$$

In the sequel we use the following expansion of a function $f \in C^s[0,1]$ in Bernoulli polynomias for any $x \in [0,1]$ (see Krylov [15, p. 15])

$$f(x) = \int_0^1 f(t)\,\mathrm{d}t + \sum_{j=1}^{s-1} \frac{B_j(x)}{j!}\left[f^{(j-1)}(1) - f^{(j-1)}(0)\right] - \frac{1}{s!}\int_0^1 f^{(s)}(t) L_s(x,t)\,\mathrm{d}t, \tag{2.4}$$

where $L_s(x,t) = B_s^*(x-t) - B_s^*(x)$ and $B_s^*(x)$ is a function of period one, defined by

$$B_s^*(x) = B_s(x), \quad 0 \le x < 1, \quad B_s^*(x+1) = B_s^*(x). \tag{2.5}$$

Notice that $B_0^*(x) = 1$, $B_1^*(x)$ is a discontinuous function with a jump of -1 at each integer, and $B_s^*(x)$, $s > 1$, is a continuous function.

Now, we can prove the following composite formula for the integral $I_n f = \int_0^n f(t)\,\mathrm{d}t$.

Theorem 2.1 *For $n, m, r \in \mathbb{N}$ $(m \le r)$ and $f \in C^{2r}[0,n]$ we have*

$$G_m^{(n)} f - I_n f = \sum_{j=m}^{r} \frac{Q_m^G(B_{2j})}{(2j)!}\left[f^{(2j-1)}(n) - f^{(2j-1)}(0)\right] + E_{n,m,r}^G(f), \tag{2.6}$$

where $G_m^{(n)} f$ is given by (2.3), *and $Q_m^G B_{2j}$ denotes the basic Gauss-Legendre quadrature sum applied to the Bernoulli polynomial $x \mapsto B_{2j}(x)$, i.e.,*

$$Q_m^G(B_{2j}) = \sum_{\nu=1}^{m} w_\nu^G B_{2j}(\tau_\nu^G) = -R_m^G(B_{2j}), \tag{2.7}$$

where $R_m^G(f)$ *is the remainder term in* (2.1).

If $f \in C^{2r+2}[0,n]$ *then there exists* $\xi \in (0,n)$, *such that the error term in* (2.6) *can be expressed in the form*

$$E_{n,m,r}^G(f) = n\,\frac{Q_m^G(B_{2r+2})}{(2r+2)!} f^{(2r+2)}(\xi). \tag{2.8}$$

P r o o f. Suppose that $f \in C^{2r}[0,n]$, where $r \geq m$.

Since the all nodes $\tau_\nu = \tau_\nu^G$, $\nu = 1,\ldots,m$, of the Gaussian rule (2.1) belong to $(0,1)$, using (2.4) with $x = \tau_\nu$ and $s = 2r+1$, we have

$$\begin{aligned} f(\tau_\nu) = I_1 f &+ \sum_{j=1}^{2r} \frac{B_j(\tau_\nu)}{j!}\left[f^{(j-1)}(1) - f^{(j-1)}(0)\right] \\ &- \frac{1}{(2r+1)!}\int_0^1 f^{(2r+1)}(t) L_{2r+1}(\tau_\nu, t)\,\mathrm{d}t, \end{aligned}$$

from which, by multiplying by $w_\nu = w_\nu^G$ and summing in ν from 1 to m, we get

$$\begin{aligned} \sum_{\nu=1}^m w_\nu f(\tau_\nu) \quad = \quad & \left(\sum_{\nu=1}^m w_\nu\right)\int_0^1 f(t)\,\mathrm{d}t \\ & + \sum_{j=1}^{2r} \frac{1}{j!}\left(\sum_{\nu=1}^m w_\nu B_j(\tau_\nu)\right)\left[f^{(j-1)}(1) - f^{(j-1)}(0)\right] \\ & - \frac{1}{(2r+1)!}\int_0^1 f^{(2r+1)}(t)\left(\sum_{\nu=1}^m w_\nu L_{2r+1}(\tau_\nu, t)\right)\mathrm{d}t, \end{aligned}$$

i.e.,

$$Q_m^G f = Q_m^G(1)\int_0^1 f(t)\,\mathrm{d}t + \sum_{j=1}^{2r}\frac{Q_m^G(B_j)}{j!}\left[f^{(j-1)}(1) - f^{(j-1)}(0)\right] + E_{m,r}^G(f),$$

where

$$E_{m,r}^G(f) = -\frac{1}{(2r+1)!}\int_0^1 f^{(2r+1)}(t) Q_m^G\left(L_{2r+1}(\,\cdot\,,t)\right)\mathrm{d}t.$$

Since

$$\int_0^1 B_j(x)\,\mathrm{d}x = \begin{cases} 1, & j = 0, \\ 0, & j \geq 1, \end{cases}$$

and

$$Q_m^G(B_j) = \sum_{\nu=1}^{m} w_\nu B_j(\tau_\nu) = \begin{cases} 1, & j = 0, \\ 0, & 1 \le j \le 2m-1, \end{cases}$$

because the Gauss-Legendre formula is exact for all algebraic polynomials of degree at most $2m-1$, the previous formula becomes

$$Q_m^G f - \int_0^1 f(t)\,\mathrm{d}t = \sum_{j=2m}^{2r} \frac{Q_m^G(B_j)}{j!}\left[f^{(j-1)}(1) - f^{(j-1)}(0)\right] + E_{m,r}^G(f). \quad (2.9)$$

Notice that for Gauss-Legendre nodes and weights the following equalities

$$\tau_\nu + \tau_{m-\nu+1} = 1, \quad w_\nu = w_{m-\nu+1} > 0, \quad \nu = 1, \ldots, m,$$

hold, as well as

$$w_\nu B_j(\tau_\nu) + w_{m-\nu+1} B_j(\tau_{m-\nu+1}) = w_\nu B_j(\tau_\nu)(1 + (-1)^j),$$

which is equal to zero for odd j. Also, if m is odd, then $\tau_{(m+1)/2} = 1/2$ and $B_j(1/2) = 0$ for each odd j. Thus, the quadrature sum

$$Q_m^G(B_j) = \sum_{\nu=1}^{m} w_\nu B_j(\tau_\nu) = 0$$

for odd j, so that (2.9) becomes

$$Q_m^G f - \int_0^1 f(t)\,\mathrm{d}t = \sum_{j=m}^{r} \frac{Q_m^G(B_{2j})}{(2j)!}\left[f^{(2j-1)}(1) - f^{(2j-1)}(0)\right] + E_{m,r}^G(f). \quad (2.10)$$

Now, for the (shifted) composite Gauss-Legendre formula we have

$$\begin{aligned} G_m^{(n)} f - I_n f &= \sum_{k=0}^{n-1} \left[Q_m^G f(k + \cdot\,) - \int_k^{k+1} f(t)\,\mathrm{d}t\right] \\ &= \sum_{k=0}^{n-1} \left[Q_m^G f(k + \cdot\,) - \int_0^1 f(k+x)\,\mathrm{d}x\right]. \end{aligned}$$

Finally, using (2.10) we obtain

$$G_m^{(n)} f - I_n f = \sum_{k=0}^{n-1} \left\{ \sum_{j=m}^{r} \frac{Q_m^G(B_{2j})}{(2j)!}\left[f^{(2j-1)}(k+1) - f^{(2j-1)}(k)\right]\right.$$

$$\begin{aligned} & +E^G_{m,r}(f(k+\,\cdot\,))\Big\} \\ = & \sum_{j=m}^{r} \frac{Q^G_m(B_{2j})}{(2j)!}\left[f^{(2j-1)}(n)-f^{(2j-1)}(0)\right]+E^G_{n,m,r}(f), \end{aligned}$$

where $E^G_{n,m,r}(f)$ is given by

$$E^G_{n,m,r}(f) = -\frac{1}{(2r+1)!}\int_0^1 \Bigg(\sum_{k=0}^{n-1} f^{(2r+1)}(k+t)\Bigg) Q^G_m\left(L_{2r+1}(\,\cdot\,,t)\right)\,\mathrm{d}t. \quad (2.11)$$

Since $L_{2r+1}(x,t) = B^*_{2r+1}(x-t) - B^*_{2r+1}(x)$ and

$$B^*_{2r+1}(\tau_\nu) = B_{2r+1}(\tau_\nu), \quad B^*_{2r+1}(\tau_\nu - t) = -\frac{1}{2r+2}\frac{\mathrm{d}}{\mathrm{d}t}B^*_{2r+2}(\tau_\nu - t),$$

we have

$$\begin{aligned} Q^G_m\left(L_{2r+1}(\,\cdot\,,t)\right) &= Q^G_m\left(B^*_{2r+1}(\,\cdot\,-t)\right) - Q^G_m\left(B^*_{2r+1}(\,\cdot\,)\right) \\ &= -\frac{1}{2r+2}\,Q^G_m\left(\frac{\mathrm{d}}{\mathrm{d}t}B^*_{2r+2}(\,\cdot\,-t)\right), \end{aligned}$$

because $Q^G_m\left(B_{2r+1}(\,\cdot\,)\right) = 0$. Then for (2.11) we get

$$(2r+2)!E^G_{n,m,r}(f) = \int_0^1 \Bigg(\sum_{k=0}^{n-1} f^{(2r+1)}(k+t)\Bigg) Q^G_m\left(\frac{\mathrm{d}}{\mathrm{d}t}B^*_{2r+2}(\,\cdot\,-t)\right)\,\mathrm{d}t.$$

By using an integration by aprts, the right-hand side reduces to

$$RHS = F(t)Q^G_m\left(B^*_{2r+2}(\,\cdot\,-t)\right)\Big|_0^1 - \int_0^1 Q^G_m\left(B^*_{2r+2}(\,\cdot\,-t)\right)F'(t)\,\mathrm{d}t,$$

where

$$F(t) = \sum_{k=0}^{n-1} f^{(2r+1)}(k+t).$$

Since $B^*_{2r+2}(\tau_\nu - 1) = B^*_{2r+2}(\tau_\nu) = B_{2r+2}(\tau_\nu)$, we have

$$\begin{aligned} F(t)Q^G_m\left(B^*_{2r+2}(\,\cdot\,-t)\right)\Big|_0^1 &= (F(1)-F(0))Q^G_m\left(B^*_{2r+2}(\,\cdot\,)\right) \\ &= Q^G_m\left(B_{2r+2}(\,\cdot\,)\right)\int_0^1 F'(t)\,\mathrm{d}t, \end{aligned}$$

so that

$$RHS = \int_0^1 \left[Q_m^G \left(B_{2r+2}(\,\cdot\,) \right) - Q_m^G \left(B_{2r+2}^*(\,\cdot\, - t) \right) \right] F'(t)\, \mathrm{d}t.$$

Since

$$(-1)^{r-m} Q_m^G \left[B_{2r+2}(\,\cdot\,) - B_{2r+2}^*(\,\cdot\, - t) \right] > 0, \qquad 0 < t < 1, \tag{2.12}$$

there exists an $\eta \in (0,1)$ such that

$$RHS = F'(\eta) \int_0^1 Q_m^G \left[B_{2r+2}(\,\cdot\,) - B_{2r+2}^*(\,\cdot\, - t) \right] \mathrm{d}t.$$

Because of continuity of $f^{(2r+2)}$ on $[0,n]$ we conclude that there exists also $\xi \in (0,n)$ such that $F'(\eta) = n f^{(2r+2)}(\xi)$.

Because of $\int_0^1 Q_m^G \left[B_{2r+2}^*(\,\cdot\, - t) \right] \mathrm{d}t = 0$, we finally obtain that

$$(2r+2)! E_{n,m,r}^G(f) = n f^{(2r+2)}(\xi) \int_0^1 Q_m^G \left[B_{2r+2}(\,\cdot\,) \right] \mathrm{d}t,$$

i.e., (2.8). □

Remark 2.1 Let $g_{m,r}^G(t)$ be the left-hand side in (2.12). Typical graphs of functions $g_{m,r}^G(t)$ for some selected values of $r \geq m \geq 1$ are presented in Figure 2.1.

Now we consider some special cases of the formula (2.6) for some typical values of m. For a given m, by $G^{(m)}$ we denote the sequence of coefficients which appear in the sum on the right-hand side in (2.6), i.e.,

$$G^{(m)} = \{ Q_m^G(B_{2j}) \}_{j=m}^{\infty} = \left\{ Q_m^G(B_{2m}), Q_m^G(B_{2m+2}), Q_m^G(B_{2m+4}), \ldots \right\}.$$

These Gaussian sums we can calculate very easy by using Mathematica Package `OrthogonalPolynomials`. In the sequel we mention cases when $1 \leq m \leq 7$.

Case $m = 1$. Here $\tau_1^G = 1/2$ and $w_1^G = 1$, so that, according to (2.7),

$$Q_1^G(B_{2j}) = B_{2j}(1/2) = (2^{1-2j} - 1) B_{2j},$$

and (2.6) reduces to (1.7). Thus,

$$G^{(1)} = \left\{ -\frac{1}{12}, \frac{7}{240}, -\frac{31}{1344}, \frac{127}{3840}, -\frac{2555}{33792}, \frac{1414477}{5591040}, -\frac{57337}{49152}, \frac{118518239}{16711680}, \ldots \right\}.$$

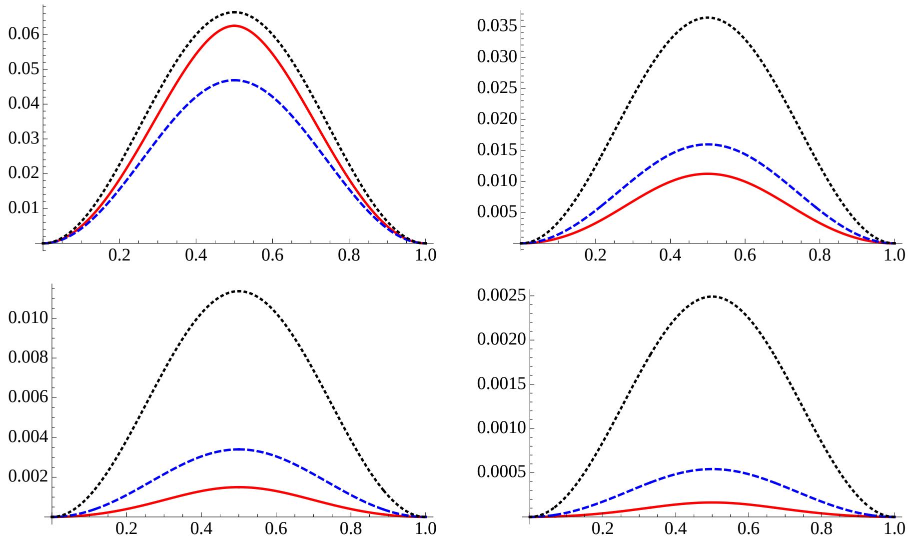

Fig. 2.1. Graphs of $t \mapsto g_{m,r}^G(t)$, $r = m$ (solid line), $r = m+1$ (dashed line), and $r = m+2$ (dotted line), when $m = 1$, $m = 2$ (top), and $m = 3$, $m = 4$ (bottom)

Case $m = 2$. Here

$$\tau_1^G = \frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right), \quad \tau_2^G = \frac{1}{2}\left(1 + \frac{1}{\sqrt{3}}\right) \quad \text{and} \quad w_1^G = w_2^G = \frac{1}{2},$$

so that

$$Q_2^G(B_{2j}) = \frac{1}{2}\left(B_{2j}(\tau_1^G) + B_{2j}(\tau_2^G)\right) = B_{2j}(\tau_1^G).$$

In this case, the sequence of coefficients is

$$G^{(2)} = \left\{-\frac{1}{180}, \frac{1}{189}, -\frac{17}{2160}, \frac{97}{5346}, -\frac{1291411}{21228480}, \frac{16367}{58320}, -\frac{243615707}{142767360}, \dots\right\}.$$

Case $m = 3$. Here

$$\tau_1^G = \frac{1}{10}\left(5 - \sqrt{15}\right), \quad \tau_2^G = \frac{1}{2}, \quad \tau_3^G = \frac{1}{10}\left(5 + \sqrt{15}\right)$$

$$w_1^G = \frac{5}{18}, \quad w_2^G = \frac{4}{9}, \quad w_3^G = \frac{5}{18},$$

so that

$$Q_3^G(B_{2j}) = \frac{5}{9} B_{2j}(\tau_1^G) + \frac{4}{9} B_{2j}(\tau_2^G)$$

and

$$G^{(3)} = \left\{-\frac{1}{2800}, \frac{49}{72000}, -\frac{8771}{5280000}, \frac{4935557}{873600000}, -\frac{15066667}{576000000}, \frac{3463953717}{21760000000}, \ldots\right\}.$$

Case $m = 4$. The corresponding sequence of coefficients is

$$G^{(4)} = \left\{-\frac{1}{44100}, \frac{41}{565950}, -\frac{3076}{11704875}, \frac{93553}{75631500}, -\frac{453586781}{60000990000}, \ldots\right\}.$$

Case $m = 5$. Here

$$G^{(5)} = \left\{-\frac{1}{698544}, \frac{205}{29719872}, -\frac{100297}{2880541440}, \frac{76404959}{352578272256}, \ldots\right\}.$$

Case $m = 6$. Here

$$G^{(6)} = \left\{-\frac{1}{11099088}, \frac{43}{70436520}, -\frac{86221}{21074606784}, \frac{147502043}{4534139665440}, \ldots\right\}.$$

Case $m = 7$. Here

$$G^{(7)} = \left\{-\frac{1}{176679360}, \frac{1603}{31236910848}, -\frac{14669711}{33282622264320}, +\frac{5003171345}{1147724953030656}, \ldots\right\}.$$

3. *Euler-Maclaurin formula based on the composite Lobatto formula*

We can also consider the corresponding Gauss-Lobatto quadrature formula

$$\int_0^1 f(x)\,\mathrm{d}x = \sum_{\nu=0}^{m+1} w_\nu^L f(\tau_\nu^L) + R_m^L(f), \tag{3.1}$$

with the nodes $\tau_0 = \tau_0^L = 0$, $\tau_{m+1} = \tau_{m+1}^L = 1$, and others internal nodes $\tau_\nu = \tau_\nu^L$, $\nu = 1, \ldots, m$, which are zeros of the shifted (monic) Jacobi polynomial,

$$\pi_m(x) = \binom{2m+2}{m}^{-1} P_m^{(1,1)}(2x-1),$$

orthogonal on the interval $(0,1)$ with respect to the weight function $x \mapsto x(1-x)$. Degree of its algebraic precision is $d = 2m+1$, i.e., $R_m^L(f) = 0$ for all algebraic polynomials of degree $\le 2m+1$.

In construction of the Gauss-Lobatto formula

$$Q_m^L(f)=\sum_{\nu=0}^{m+1} w_\nu^L f(\tau_\nu^L), \tag{3.2}$$

we can use parameters of the corresponding Gaussian formula

$$\int_0^1 g(x)x(1-x)\,\mathrm{d}x=\sum_{\nu=1}^{m}\widehat{w}_\nu^G g(\widehat{\tau}_\nu^G)+\widehat{R}_m^G(g),$$

which can be calculated from an eigenvalue problem for the symmetric tridiagonal Jacobi matrix (2.2), in this case, with the three-term recurrence coefficients,

$$\widehat{\alpha}_k=1/2,\quad \widehat{\beta}_k=\frac{1}{4}\cdot\frac{k(k+2)}{(2k+1)(2k+3)},\quad k\in\mathbb{N}.$$

The nodes of the Gauss-Lobatto quadrature formula (3.1) are $\tau_0^L=0$, $\tau_\nu^L=\widehat{\tau}_\nu^G$, $\nu=1,\ldots,m$, $\tau_{m+1}^L=1$, and the corresponding weights (cf. [18, pp. 330–331]) are

$$w_\nu^L=\frac{\widehat{w}_\nu^G}{\widehat{\tau}_\nu^G(1-\widehat{\tau}_\nu^G)},\quad \nu=1,\ldots,m,$$

and

$$w_0^L=\frac{1}{2}-\sum_{\nu=1}^{m}\frac{\widehat{w}_\nu^G}{\widehat{\tau}_\nu^G},\quad w_{m+1}^L=\frac{1}{2}-\sum_{\nu=1}^{m}\frac{\widehat{w}_\nu^G}{1-\widehat{\tau}_\nu^G}.$$

The corresponding composite rule is

$$L_m^{(n)}f=\sum_{k=0}^{n-1}Q_m^L f(k+\cdot)=\sum_{\nu=0}^{m+1}w_\nu^L\sum_{k=0}^{n-1}f(k+\tau_\nu^L),$$

i.e.,

$$L_m^{(n)}f=(w_0^L+w_{m+1}^L){\sum_{k=0}^{n}}'' f(k)+\sum_{\nu=1}^{m}w_\nu^L\sum_{k=0}^{n-1}f(k+\tau_\nu^L). \tag{3.3}$$

As in the Gauss-Legendere case, there exists a symmetry of nodes and weights, i.e.,

$$\tau_\nu^L+\tau_{m+1-\nu}^L=1,\quad w_\nu^L=w_{m+1-\nu}^L>0,\quad \nu=0,1,\ldots,m+1,$$

so that the Gauss-Lobatto quadrature sum

$$Q_m^L(B_j)=\sum_{\nu=0}^{m+1}w_\nu^L B_j(\tau_\nu^L)=0$$

for each odd j.

Using the same arguments as before, we can state and prove the following result.

Theorem 3.1 *For $n, m, r \in \mathbb{N}$ $(m \le r)$ and $f \in C^{2r}[0,n]$ we have*

$$L_m^{(n)} f - I_n f = \sum_{j=m+1}^{r} \frac{Q_m^L(B_{2j})}{(2j)!} \left[f^{(2j-1)}(n) - f^{(2j-1)}(0) \right] + E_{n,m,r}^L(f), \quad (3.4)$$

where $L_m^{(n)} f$ is given by (3.3), *and $Q_m^L B_{2j}$ denotes the basic Gauss-Lobatto quadrature sum* (3.2) *applied to the Bernoulli polynomial $x \mapsto B_{2j}(x)$, i.e.,*

$$Q_m^L(B_{2j}) = \sum_{\nu=0}^{m+1} w_\nu^L B_{2j}(\tau_\nu^L) = -R_m^L(B_{2j}),$$

where $R_m^L(f)$ is the remainder term in (3.1).

If $f \in C^{2r+2}[0,n]$ then there exists $\xi \in (0,n)$, such that the error term in (3.4) *can be expressed in the form*

$$E_{n,m,r}^L(f) = n\, \frac{Q_m^L(B_{2r+2})}{(2r+2)!} f^{(2r+2)}(\xi).$$

Remark 3.1 As in Remark 2.1 we have $g_{m,r}^L(t) > 0$ for $0 < t < 1$, where

$$g_{m,r}^L(t) := (-1)^{r-m} Q_m^L \left[B_{2r+2}(\,\cdot\,) - B_{2r+2}^*(\,\cdot\, - t) \right].$$

Typical graphs of $g_{m,r}^L(t)$ for some selected values of $r \ge m+1 \ge 1$ are presented in Figure 3.1.

In the sequel we give the sequence of coefficients $L^{(m)}$ which appear in the sum on the right-hand side in (3.4), i.e.,

$$L^{(m)} = \{Q_m^L(B_{2j})\}_{j=m+1}^{\infty} = \left\{ Q_m^L(B_{2m+2}), Q_m^L(B_{2m+4}), Q_m^L(B_{2m+6}), \ldots \right\},$$

obtained by using Mathematica Package `OrthogonalPolynomials`, for some typical values of m.

Case $m = 0$. This is a case of the standard Euler-Maclaurin formula (1.1), for which $\tau_0^L = 0$ and $\tau_1^L = 1$, with $w_0^L = w_1^L = 1/2$. The sequence of coefficients is

$$L^{(0)} = \left\{ \frac{1}{6}, -\frac{1}{30}, \frac{1}{42}, -\frac{1}{30}, \frac{5}{66}, -\frac{691}{2730}, \frac{7}{6}, -\frac{3617}{510}, \frac{43867}{798}, -\frac{174611}{330}, \frac{854513}{138}, \ldots \right\},$$

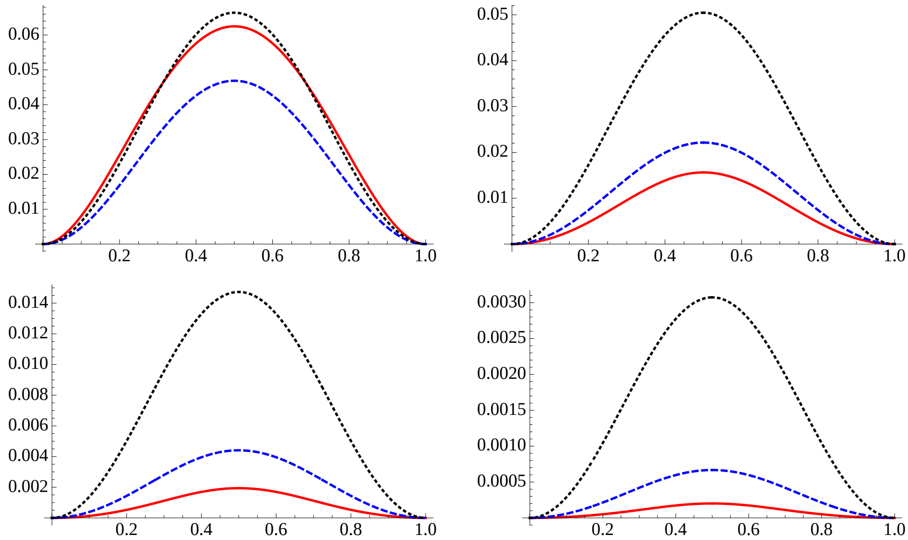

Fig. 3.1. Graphs of $t \mapsto g_{m,r}^L(t)$, $r = m+1$ (solid line), $r = m+2$ (dashed line), and $r = m+3$ (dotted line), when $m = 0$, $m = 1$ (top), and $m = 2$, $m = 3$ (bottom)

which is, in fact, the sequence of Bernoulli numbers $\{B_{2j}\}_{j=1}^{\infty}$.

Case $m = 1$. In this case $\tau_0^L = 0$, $\tau_1^L = 1/2$, and $\tau_2 = 1$, with the corresponding weights $w_0^L = 1/6$, $w_1^L = 2/3$, and $w_2^L = 1/6$, which is, in fact, the Simpson formula (1.8). The sequence of coefficients is

$$L^{(1)} = \left\{\frac{1}{120}, -\frac{5}{672}, \frac{7}{640}, -\frac{425}{16896}, \frac{235631}{2795520}, -\frac{3185}{8192}, \frac{19752437}{8355840}, -\frac{958274615}{52297728}, \dots\right\}.$$

Case $m = 2$. Here

$$\tau_0^L = 0, \quad \tau_1^L = \frac{1}{10}(5-\sqrt{5}), \quad \tau_2^L = \frac{1}{10}(5+\sqrt{5}), \quad \tau_3^L = 1$$

and $w_0^L = w_3^L = 1/12$, $w_1^L = w_2^L = 5/12$, and the sequence of coefficients is

$$L^{(2)} = \left\{\frac{1}{2100}, -\frac{1}{1125}, \frac{89}{41250}, -\frac{25003}{3412500}, \frac{3179}{93750}, -\frac{2466467}{11953125}, \frac{997365619}{623437500}, \dots\right\}.$$

Case $m = 3$. Here

$$\tau_0^L = 0, \quad \tau_1^L = \frac{1}{14}(7-\sqrt{31}), \quad \tau_2^L = \frac{1}{2}, \quad \tau_3^L = \frac{1}{14}(7+\sqrt{31}), \quad \tau_4^L = 1$$

and

$$w_0^L = \frac{1}{20}, \quad w_1^L = \frac{49}{180}, \quad w_2^L = \frac{16}{45}, \quad w_3^L = \frac{49}{180}, \quad w_4^L = \frac{1}{20},$$

and the sequence of coefficients is

$$L^{(3)} = \left\{ \frac{1}{35280}, -\frac{65}{724416}, \frac{38903}{119857920}, -\frac{236449}{154893312}, \frac{1146165227}{122882027520}, \dots \right\}.$$

Case $m = 4$. The corresponding sequence of coefficients is

$$L^{(4)} = \left\{ \frac{1}{582120}, -\frac{17}{2063880}, \frac{173}{4167450}, -\frac{43909}{170031960}, \frac{160705183}{79815002400}, \dots \right\}.$$

Case $m = 5$. Here

$$L^{(5)} = \left\{ \frac{1}{9513504}, -\frac{49}{68999040}, \frac{5453}{1146917376}, -\frac{671463061}{17766424811520}, \dots \right\}.$$

Case $m = 6$. In this case the corresponding sequence of coefficients is

$$L^{(6)} = \left\{ \frac{1}{154594440}, -\frac{50}{854134281}, \frac{16331}{32502560805}, -\frac{19490189}{3922888023054}, \dots \right\}.$$

Case $m = 7$. Here

$$L^{(7)} = \left\{ \frac{1}{2502957600}, -\frac{29}{6216496000}, \frac{89209}{1786424640000}, -\frac{776272933}{1291329811200000}, \dots \right\}.$$

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