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Euler–Maclaurin Expansions for Integrals over Triangles and Squares of Functions Having Algebraic/Logarithmic Singularities along an Edge

AVRAM SIDI

Computer Science Department, Technion, Haifa 32000, Israel

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We derive and analyze the properties of Euler–Maclaurin expansions for the differences $\int_S\int x^s(\log x)^{s'} f(x,y) - Q_h^S[f]$, $s > -1$, $s' = 0, 1$, where S denotes either the simplex $\{(x,y) | x+y \leqslant 1, x \geqslant 0, y \geqslant 0\}$ or the square $\{(x,y) | 0 \leqslant x \leqslant 1, 0 \leqslant y \leqslant 1\}$, and $Q_h^S[f]$ is a combination of one-dimensional generalized trapezoidal rule approximations.

1. INTRODUCTION

In this work we are interested in deriving Euler–Maclaurin expansions for the singular double integrals

$$Q[f] = \int_T\int w(x) f(x,y)\,dx\,dy, \quad T = \{(x,y) | x+y \leqslant 1, x \geqslant 0, y \geqslant 0\}, \tag{1.1}$$

$$Q'[f] = \int_{T'}\int w(x) f(x,y)\,dx\,dy, \quad T' = \{(x,y) | 0 \leqslant x \leqslant 1, 0 \leqslant y \leqslant 1\}, \tag{1.2}$$

where

$$w(x) = x^s(\log x)^{s'}, \qquad s > -1, s' = 0, 1, \tag{1.3}$$

and $f(x,y)$ is as many times differentiable as needed. Specifically we are looking for asymptotic expansions, as $h \to 0+$, for the differences $\Delta_h[f] = Q[f] - Q_h[f]$ and $\Delta'_h[f] = Q'[f] - Q'_h[f]$, where $Q_h[f]$ and $Q'_h[f]$ are approximations to $Q[f]$ and $Q'[f]$, respectively, obtained as some combinations of one-dimensional generalized trapezoidal rule approximations with step size h.

We now state some results which bear relevance to our derivation of the Euler–Maclaurin formulas for $Q[f]$ and $Q'[f]$.

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THEOREM 1.1 (See Steffensen [8, Section 14]). *Let the function $g(x)$ be $2m$ times differentiable on $[a, b]$ and let $h = (b-a)/n$, where n is a positive integer. Let ε be a fixed constant satisfying $0 \leqslant \varepsilon \leqslant 1$. Then*

$$D(h) = \int_a^b g(x)\,dx - h \sum_{j=0}^{n-1} g(a + jh + \varepsilon h)$$
$$= -\sum_{\mu=1}^{2m-1} \frac{B_\mu(\varepsilon)}{\mu!} [g^{(\mu-1)}(b) - g^{(\mu-1)}(a)]\, h^\mu$$
$$+ R_{2m}[g; (a, b)], \tag{1.4}$$

where

$$R_{2m}[g; (a, b)] = h^{2m} \int_a^b \frac{\bar{B}_{2m}[\varepsilon - (x-a)/h] - B_{2m}(\varepsilon)}{(2m)!} g^{(2m)}(x)\,dx. \tag{1.5}$$

Here $B_\mu(x)$ is the Bernoulli polynomial of degree μ and $\bar{B}_\mu(x)$ is the periodic Bernoullian function of order μ.

Since $\bar{B}_\mu(x)$ are bounded on $(-\infty, \infty)$, it follows that

$$|R_{2m}[g; (a, b)(a, b)]| \leqslant M_{2m}(b-a)\, h^{2m} \max_{a \leqslant x \leqslant b} |g^{(2m)}(x)|, \tag{1.6}$$

where

$$M_{2m} = \max_{-\infty < x < \infty} |\bar{B}_{2m}(\varepsilon + x) - B_{2m}(\varepsilon)|/(2m)! \tag{1.7}$$

and, therefore, is independent of h. Consequently, if $g(x)$ is infinitely differentiable on $[a, b]$, then $D(h)$ has an asymptotic expansion of the form

$$D(h) \sim \sum_{\mu=1}^{\infty} \frac{B_\mu(\varepsilon)}{\mu!} [g^{(\mu-1)}(a) - g^{(\mu-1)}(b)]\, h^\mu \quad \text{as } h \to 0+. \tag{1.8}$$

The following result is due to Navot [4]. See also Navot [5].

THEOREM 1.2. *Let the function $g(x)$ be $2m$ times differentiable on $[0, 1]$ and let $G(x) = x^s g(x)$ for $-1 < s < 0$. Let $h = 1/n$, where n is a positive integer. Then for $0 < \varepsilon \leqslant 1$,*

$$D(h) = \int_0^1 G(x)\,dx - h \sum_{j=0}^{n-1} G(jh + \varepsilon h)$$
$$= -\sum_{\mu=1}^{2m-1} \frac{B_\mu(\varepsilon)}{\mu!} G^{(\mu-1)}(1)\, h^\mu - \sum_{\mu=0}^{2m-1} \frac{\zeta(-s-\mu, \varepsilon)}{\mu!}$$
$$\times g^{(\mu)}(0)\, h^{\mu+s+1} + \rho_{2m}, \tag{1.9}$$

where $\zeta(t, \varepsilon)$ *is the generalized Riemann zeta function initially defined for* $\operatorname{Re} t > 1$ *by* $\zeta(t, \varepsilon) = \sum_{k=0}^{\infty} (k+\varepsilon)^{-t}$, *and then continued analytically, and*

$$\rho_{2m} = 0(h^{2m}) \qquad \textit{as} \quad h \to 0+. \tag{1.10}$$

Noting that $\zeta(-j, \varepsilon) = -B_{j+1}(\varepsilon)/(j+1)$, $j = 0, 1, \ldots$, Navot [4] shows that (1.9) reduces to (1.4) in the limit $s \to 0$.

Remark. The result of Theorem 1.2 holds also for $s > 0$ since for this case the integrand can be written in the form $G(x) = x^r u(x)$, where $-1 < r \leqslant 0$ and $u(x)$ is at least as smooth as $g(x)$ at $x = 0$. Actually $r = s - \bar{s}$ and $u(x) = x^{\bar{s}} g(x)$, where $\bar{s}$ is the smallest integer greater than or equal to s. It is clear that $u^{(i)}(0) = 0$, for $0 \leqslant i \leqslant \bar{s} - 1$, hence the sum that contains the zeta functions in (1.9) becomes $\sum_{\nu=0}^{2m-\bar{s}-1} (\zeta(-s-\nu, \varepsilon)/\nu!)\, g^{(\nu)}(0)\, h^{\nu+s+1}$ which is simply $\sum_{\nu=0}^{2m-1} (\zeta(-s-\nu, \varepsilon)/\nu!)\, g^{(\nu)}(0)\, h^{\nu+s+1} + 0(h^{2m})$ as $h \to 0+$, since the terms with $\nu \geqslant 2m - \bar{s}$ in the last summation are $0(h^{2m})$ as $h \to 0$. The summation that contains the Bernoulli polynomials stays the same. Finally, when $g(x)$ is infinitely differentiable on $[0, 1]$, $D(h)$ has the asymptotic expansion

$$D(h) = -\sum_{\mu=1}^{\infty} \frac{B_\mu(\varepsilon)}{\mu!} G^{(\mu-1)}(1)\, h^\mu - \sum_{\mu=0}^{\infty} \frac{\zeta(-s-\mu, \varepsilon)}{\mu!} g^{(\mu)}(0)\, h^{\mu+s+1}$$
$$\text{as} \quad h \to 0+, \tag{1.11}$$

for *all* $s > -1$.

Starting with Theorem 1.2, Navot [5] proves the following:

THEOREM 1.3. *If in Theorem* 1.2 *we let* $G(x) = g(x)\, x^s \log x$, $-1 < s < 0$, *then*

$$D(h) = \sum_{\mu=1}^{2m-1} \alpha_\mu h^\mu + \log h \sum_{\mu=0}^{2m-1} \beta_\mu h^{\mu+s+1} + \sum_{\mu=0}^{2m-1} \gamma_\mu h^{\mu+s+1}$$
$$+\, 0(h^{2m}) \qquad \text{as} \quad h \to 0+, \tag{1.12}$$

and if we let $G(x) = g(x) \log x$, *then*

$$D(h) = \sum_{\mu=1}^{2m-1} \alpha'_\mu h^\mu + \log h \sum_{\mu=0}^{2m-1} \beta'_\mu h^{\mu+1} + 0(h^{2m}) \quad \textit{as}\ h \to 0+, \tag{1.13}$$

where α_μ, β_μ, γ_μ, α'_μ, β'_μ *are constants independent of* h *and they depend solely on* g *and its derivatives evaluated at* $x = 0$ *and* $x = 1$. (1.12) *can be obtained by formally differentiating both sides of* (1.9) *with respect to* s. (1.13) *can be obtained by letting* $s = 0$ *in* (1.12).

Remark. Like (1.9), (1.12) too can be shown to hold for all $s > -1$. Again, when $g(x)$ is infinitely differentiable on $[0, 1]$, $D(h)$ in (1.12) and (1.13) have asymptotic expansions as $h \to 0+$, similar to those given in (1.8) and (1.11).

Other facts that will be of use in the remainder of this work are

$$B_1 = B_1(0) = -B_1(1) = -\tfrac{1}{2}, \quad B_\mu = B_\mu(0) = B_\mu(1), \quad \mu = 2, 3, \ldots, \tag{1.14}$$

where B_μ are the Bernoulli numbers,

$$B_{2\mu+1} = 0, \qquad \mu = 1, 2, \ldots, \tag{1.15}$$

$$B_{2\mu+1}(\tfrac{1}{2}) = 0, \qquad \mu = 0, 1, \ldots, \tag{1.16}$$

and

$$\zeta(t, 1) = \zeta(t), \tag{1.17}$$

where $\zeta(t)$ is the Riemann zeta function.

2. Euler–Maclaurin Expansions For $Q[f]$: The Case $s' = 0$

Theorem 2.1. *Let $f(x, y)$ be $2m$ times differentiable on the simplex T defined in* (1.1), *i.e., let all partial derivatives of $f(x, y)$ of total order $\leqslant 2m$ exist and be continuous on T. Let $h = 1/n$, where n is a positive integer, and let ε be a fixed constant satisfying $0 \leqslant \varepsilon \leqslant 1$. Let $Q[f]$ be as in* (1.1) *and* (1.3) *with $s' = 0$. Define*

$$Q_h[f] = h^2 \sum_{i=1}^{n-1} (ih)^s \sum_{j=0}^{n-i-1} f(ih, jh + \varepsilon h). \tag{2.1}$$

Then

$$A_h[f] = Q[f] - Q_h[f] = \sum_{k=1}^{2m-1} a_k h^k + \sum_{k=0}^{2m-1} b_k h^{s+k+1} + \sigma_{2m}, \tag{2.2}$$

where

$$\sigma_{2m} = O(h^{2m}) \qquad as \quad h \to 0+, \tag{2.3}$$

and the coefficients a_k, b_k are independent of h. (The expressions for a_k, b_k are complicated and will be given in the proof below.)

Proof. We start by writing $Q[f]$ as an iterated integral. If we define

$$F(x) = \int_0^{1-x} f(x, y)\, dy. \tag{2.4}$$

then $Q[f]$ becomes

$$Q[f] = \int_0^1 x^s F(x)\,dx. \tag{2.5}$$

Since $f(x, y)$ is $2m$ times differentiable on T, $F(x)$ is $2m$ times differentiable on $[0, 1]$. Therefore, Theorem 1.2 applies to (2.5) and we have (taking $\varepsilon = 1$)

$$\begin{aligned} Q[f] = h \sum_{i=1}^{n-1} x^s F(x)|_{x=ih} + \sum_{k=1}^{2m-1} c_k h^k \\ + \sum_{k=0}^{2m-1} d_k h^{s+k+1} + \rho_{2m}, \end{aligned} \tag{2.6}$$

where

$$\begin{aligned} c_k &= -\frac{B_k(1)}{k!} [x^s F(x)]^{(k-1)}|_{x=1}, \qquad & k = 1, 2, \ldots, \\ d_k &= -\frac{\zeta(-s-k)}{k!} F^{(k)}(0), & k = 0, 1, \ldots \end{aligned} \tag{2.7}$$

and $\rho_{2m} = 0(h^{2m})$ as $h \to 0+$. In the first summation on the right-hand side of (2.6) the term with $i = n$ is missing since $F(nh) = F(1) = 0$. Also $c_1 = 0$ for the same reason. In (2.7) we have also used (1.17).

Let us now approximate $F(ih)$ by the generalized trapezoidal rule with step size h. This is possible since $1 - ih$ is a multiple of h. From Theorem 1.1 we then have

$$\begin{aligned} F(ih) &= \int_0^{1-ih} f(ih, y)\,dy \\ &= h \sum_{j=0}^{n-i-1} f(ih, jh + \varepsilon h) \\ &\quad - \sum_{\mu=1}^{2m-1} \frac{B_\mu(\varepsilon)}{\mu!} h^\mu \psi_{\mu-1}(ih) + \tau_{2m,i}, \end{aligned} \tag{2.8}$$

where

$$\psi_p(x) = \frac{\partial^p}{\partial y^p} f(x, y)|_{y=1-x} - \frac{\partial^p}{\partial y^p} f(x, y)|_{y=0}, \qquad p = 0, 1, \ldots, \tag{2.9}$$

and from (1.6)

$$|\tau_{2m,i}| \leqslant M_{2m}(1 - ih)\, h^{2m} \max_{(x,y) \in T} \left| \frac{\partial^{2m}}{\partial y^{2m}} f(x, y) \right|, \tag{2.10}$$

with M_{2m} as defined in (1.7).

Substituting (2.8) in the first summation on the right-hand side of (2.6), recalling (2.1), and rearranging, we obtain

$$
\begin{aligned}
h \sum_{i=1}^{n-1} x^s F(x)\big|_{x=ih} &= Q_h[f] - \sum_{\mu=1}^{2m-1} \frac{B_\mu(\varepsilon)}{\mu!} h^\mu \left[h \sum_{i=1}^{n-1} (ih)^s \psi_{\mu-1}(ih) \right] + \bar{\rho}_{2m}, \qquad (2.11)
\end{aligned}
$$

where

$$
\bar{\rho}_{2m} = h \sum_{i=1}^{n-1} (ih)^s \tau_{2m,i}, \tag{2.12}
$$

hence, from (2.10),

$$
\begin{aligned}
|\bar{\rho}_{2m}| &\leqslant M_{2m} \max_{(x,y)\in\Gamma} \left| \frac{\partial^{2m}}{\partial y^{2m}} f(x,y) \right| h^{2m} \left[h \sum_{i=1}^{n-1} (ih)^s (1-ih) \right] \\
&= 0(h^{2m}), \qquad (2.13)
\end{aligned}
$$

since

$$
h \sum_{i=1}^{n-1} (ih)^s (1-ih) = \int_0^1 x^s (1-x)\, dx + o(1) \qquad \text{as} \quad h \to 0+, \tag{2.14}
$$

from Theorem 1.2.

Now $\psi_p(x)$ is $2m-p$ times differentiable on $[0, 1]$ and $\psi_p(nh) = \psi_p(1) = 0$. Using this together with the fact that $s > -1$, and applying Theorem 1.2, this time to the term inside the square brackets in the summation on the rihgt-hand side of (2.11), we have

$$
\begin{aligned}
h \sum_{i=1}^{n-1} (ih)^s \psi_p(ih) &= \int_0^1 x^s \psi_p(x)\, dx + \sum_{\nu=1}^{2m-p-2} \frac{B_\nu(1)}{\nu!} [x^s \psi_p(x)]^{(\nu-1)}\big|_{x=1} h^\nu \\
&\quad + \sum_{\nu=0}^{2m-p-1} \frac{\zeta(-s-\nu)}{\nu!} \psi_p^{(\nu)}(0)\, h^{s+\nu+1} + \bar{\rho}_{2m,p}, \qquad (2.15)
\end{aligned}
$$

where

$$
\bar{\rho}_{2m,p} = 0(h^{2m-p-1}) \qquad \text{as} \quad h \to 0+. \tag{2.16}
$$

Note that since $\psi_p(1) = 0$, the first summation on the right-hand side of

(2.15) acually starts with $\nu = 2$. Substituting (2.15) and (2.16) in (2.11), we obtain

$$h \sum_{i=1}^{n-1} x^s F(x)|_{x=ih}$$

$$= Q_h[f] - \sum_{\mu=1}^{2m-1} \frac{B_\mu(\varepsilon)}{\mu!} \left[\int_0^1 x^s \psi_{\mu-1}(x)\, dx\right] h^\mu$$

$$- \sum_{\mu=1}^{2m-1} \sum_{\nu=1}^{2m-\mu-1} \frac{B_\mu(\varepsilon)}{\mu!} \frac{B_\nu(1)}{\nu!} [x^s \psi_{\mu-1}(x)]^{(\nu-1)}|_{x=1} h^{\mu+\nu}$$

$$- \sum_{\mu=1}^{2m-1} \sum_{\nu=0}^{2m-\mu} \frac{B_\mu(\varepsilon)}{\mu!} \frac{\zeta(-s-\nu)}{\nu!} \psi_{\mu-1}^{(\nu)}(0)\, h^{\mu+\nu+s+1} + 0(h^{2m}) \text{ as } h \to 0+. \tag{2.17}$$

Finally, substituting (2.17) in (2.6), we obtain (2.2) and (2.3). The coefficients a_k and b_k are now given by

$$a_1 = -B_1(\varepsilon) \int_0^1 x^s \psi_0(x)\, dx,$$

$$a_k = -\frac{B_k(\varepsilon)}{k!} \int_0^1 x^s \psi_{k-1}(x)\, dx$$

$$- \sum_{\substack{\mu+\nu=k \\ \mu,\nu \geqslant 1}} \frac{B_\mu(\varepsilon)}{\mu!} \frac{B_\nu}{\nu!} [x^s \psi_{\mu-1}(x)]^{(\nu-1)}|_{x=1}$$

$$- \frac{B_k}{k!} [x^s F(x)]^{(k-1)}|_{x=1}, \qquad k = 2, 3, \ldots, 2m-1,$$

$$b_0 = -\zeta(-s)\, F(0),$$

$$b_k = -\frac{\zeta(-s-k)}{k!} F^{(k)}(0)$$

$$- \sum_{\substack{\mu+\nu=k \\ \mu \geqslant 1, \nu \geqslant 0}} \frac{B_\mu(\varepsilon)}{\mu!} \frac{\zeta(-s-\nu)}{\nu!} \psi_{\mu-1}^{(\nu)}(0), \qquad k = 1, 2, \ldots, 2m-1, \tag{2.18}$$

where we have used (1.14) and $\psi_p(1) = 0$. ∎

The long expressions given in (2.18) can be put in a more compact form as follows: From (2.9), $\psi_p(x)$ can be expressed as

$$\psi_p(x) = \int_0^{1-x} \frac{\partial^{p+1}}{\partial y^{p+1}} f(x, y)\, dy, \qquad p = 0, 1, \ldots \tag{2.19}$$

Let us define $\psi_{-1}(x)$ by letting $p=-1$ in (2.19). It is clear that

$$\psi_{-1}(x) = F(x). \tag{2.20}$$

Let us also define

$$[x^s\psi_p(x)]^{(-1)} \equiv \int_0^x t^s\psi_p(t)\,dt = \theta_p(x), \qquad p=-1,0,1,\ldots \tag{2.21}$$

Then we have

$$\theta_p^{(j)}(x) = [x^s\psi_p(x)]^{(j-1)}, \qquad j=0,1,2,\ldots \tag{2.22}$$

Recalling that $B_0(x)=B_0=1$, a_k and b_k can now be expressed as

$$\begin{aligned} a_k &= -\sum_{\substack{\mu+\nu=k\\ \mu,\nu\geq 0}} \frac{B_\mu(\varepsilon)}{\mu!}\,\frac{B_\nu}{\nu!}\,\theta_{\mu-1}^{(\nu)}(1), \qquad k=1,2,\ldots,\\ b_k &= \sum_{\substack{\mu+\nu=k\\ \mu,\nu\geq 0}} \frac{B_\mu(\varepsilon)}{\mu!}\,\frac{\zeta(-s-\nu)}{\nu!}\,\psi_{\mu-1}^{(\nu)}(0), \quad k=0,1,\ldots. \end{aligned} \tag{2.23}$$

Remark. When the function $f(x,y)$ is infinitely differentiable on T, then the Euler–Maclaurin expansion in (2.2) can be continued indefinitely, and we have as $h\to 0+$, for all $s>-1$,

$$\Delta_h[f] \sim \sum_{k=1}^{\infty} a_k h^k + \sum_{k=0}^{\infty} b_k h^{s+k+1}. \tag{2.24}$$

COROLLARY. *If $f(x,y)$ is a polynomial in x and y of degree q, say, then $b_k=0$ for $k\geq q+2$, i.e., the series $\sum_{k=0}^{\infty} b_k h^{s+k+1}$ has actually a finite number of terms.*

Proof. It is not difficult to show that $\psi_p(x)$ is a polynomial in x of degree at most $q-p$, for $p=-1,0,1,\ldots,q$. Hence $\psi_p^{(\nu)}(x)\equiv 0$ for $\nu\geq q-p+1$. The result now follows easily. ∎

We now go on to investigate the nature of the a_k and b_k.

A simple analysis shows that for $p=0,1,\ldots$, $\nu=0,1,\ldots$,

$$\psi_p^{(\nu)}(x) = \left(\frac{\partial}{\partial x}-\frac{\partial}{\partial y}\right)^{\nu}\frac{\partial^p}{\partial y^p}f(x,y)\Big|_{y=1-x} - \frac{\partial^\nu}{\partial x^\nu}\,\frac{\partial^p}{\partial y^p}f(x,y)\Big|_{y=0} \tag{2.25}$$

so that

$$\psi_p^{(\nu)}(1) = \left[\left(\frac{\partial}{\partial x}-\frac{\partial}{\partial y}\right)^{\nu} - \frac{\partial^\nu}{\partial x^\nu}\right]\frac{\partial^p}{\partial y^p}f(x,y)\Big|_{(1,0)}. \tag{2.26}$$

Also

$$\int_0^1 x^s \psi_p(x)\,dx = \int_\Gamma w(x,y) \frac{\partial^p}{\partial y^p} f(x,y)\,dl, \tag{2.27}$$

where Γ is the polygonal arc joining (0, 1), (1, 0), (0, 0) in this order and $w(x,y) = x^s/\sqrt{2}$ along the line $x + y = 1$ and $w(x,y) = x^s$ along $y = 0$, and dl is the line element along Γ. Similarly it can be shown that

$$F^{(k)}(1) = -\sum_{\substack{i+j=k-1\\ i,j\geq 0}} \left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y}\right)^i \frac{\partial^j}{\partial y^j} f(x,y)|_{(1,0)}. \tag{2.28}$$

Hence we conclude that the contribution to the a_k comes from the derivatives of $f(x,y)$ at (1, 0), i.e., the corner across he line of singularities, and from certain integrals of $f(x,y)$ and its derivatives along the two sides of T on which there are no singularities. From (2.25) we have

$$\begin{aligned}\psi_p^{(r)}(0) = &\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y}\right)^r \frac{\partial^p}{\partial y^p} f(x,y)|_{(0,1)} \\ &- \frac{\partial^r}{\partial x^r} \frac{\partial^p}{\partial y^p} f(x,y)|_{(0,0)}.\end{aligned} \tag{2.29}$$

Also making the change of variable of integration $y = (1-x)\tau$ in the integral expression for $F(x)$ given in (2.4), and differentiating k times with respect to x, we obtain

$$F^{(k)}(x) = \int_0^1 [(1-x)\,D_\tau^k - kD_\tau^{k-1}]\,f(x,(1-x)\,\tau)\,d\tau. \tag{2.30}$$

where we have defined $D_\tau = \partial/\partial x - \tau\partial/\partial y$. Setting now $x = 0$ in (2.30) we obtain

$$F^{(k)}(0) = \int_0^1 (D^k - kD^{k-1}) f(x,y)|_{x=0}\,dy, \tag{2.31}$$

where $D = \partial/\partial x - y\partial/\partial y$. Therefore, we conclude that the contribution to the b_k comes from $f(x,y)$ and its derivatives at the points (0, 0) and (0, 1) and their integrals along the line of singularities $x = 0$.

Some special cases. (a) $\varepsilon = \frac{1}{2}$. Substituting (1.16) in (2.23) it is clear that $a_k = 0$, $k = 1, 3, 5, \ldots$, but none of the b_k's vanish in general.

(b) $\varepsilon = 1$. If we substitute (1.15) in (2.23) we realize that in general none of the a_k's are zero. However, if $Q_h[f]$ in (2.1) is modified to read

$$\bar{Q}_h[f] = h^2 \sum_{i=1}^{n-1}{}' (ih)^s \sum_{j=0}^{n-i}{}'' f(ih, jh), \tag{2.32}$$

where $\sum''^{N}_{j=0} \alpha_j = \sum^{N-1}_{j=1} \alpha_j + (\alpha_0 + \alpha_N)/2$, then using the same techniques as before, it can be shown that

$$\bar{\Delta}_h[f] = Q[f] - \bar{Q}_h[f] = \sum_{\mu=1}^{m-1} \bar{a}_{2\mu} h^{2\mu} + \sum_{\mu=0}^{2m-1} \bar{b}_\mu h^{\mu+s+1} + O(h^{2m})$$
$$\text{as} \quad h \to 0+, \tag{2.33}$$

where $\bar{a}_{2\mu}$ and $\bar{b}_k$ are as given in (2.23) with $\varepsilon = 1$, except that the terms with $\mu = 1$ are omitted in both summations.

3. Euler–Maclaurin Expansions for $Q[f]$: The Case $s' = 1$

In this section we state without proof the Euler–Maclaurin expansions for the case $s' = 1$. Letting $w(x) = x^s \log x$, we now define $Q_h[f]$ by

$$Q_h[f] = h^2 \sum_{i=1}^{n-1}{}' w(ih) \sum_{j=0}^{n-i-1}{}' f(ih, jh + \varepsilon h), \tag{3.1}$$

where $h = 1/n$, n a positive integer.

Theorem 3.1. *Let $f(x, y)$ be infinitely differentiable on T and let $Q[f]$ be as in* (1.1) *with $s' = 1$, i.e., $w(x) = x^s \log x$. Then as $h \to 0+$,*

$$Q[f] - Q_h[f] \sim \sum_{\mu=1}^{\infty}{}' a'_\mu h^\mu + \log h \sum_{\mu=0}^{\infty}{}' b'_\mu h^{\mu+s+1} + \sum_{\mu=0}^{\infty}{}' c'_\mu h^{\mu+s+1}, \tag{3.2}$$

where a'_μ, b'_μ, and c'_μ are constants independent of h.

Theorem 3.2. *Let $f(x, y)$ be infinitely differentiable on T and let $Q[f]$ be as in* (1.1) *with $s = 0$, $s' = 1$, i.e., $w(x) = \log x$. Then as $h \to 0+$,*

$$Q[f] - Q_h[f] \sim \sum_{\mu=1}^{\infty}{}' a''_\mu h^\mu + \log h \sum_{\mu=0}^{\infty}{}' b''_\mu h^{\mu+1}, \tag{3.3}$$

where a''_μ and b''_μ are constants independent of h.

The proofs of these two theorems are exactly the same as that of Theorem 2.1, the only difference being that use is made of Theorem 1.3 with (1.12) and (1.13), respectively, instead of Theorem 1.2. Expressions for a'_μ, b'_μ, c'_μ, a''_μ, and b''_μ can be found in terms of $f(x, y)$ and its derivatives and their integrals but this will be omitted here.

We shall only state that (3.2) can be formally obtained by differentiating both sides of (2.24) with respect to s. (3.3) is then obtained by letting $s = 0$ on both sides of (3.2). When $f(x, y)$ is a polynomial in x and y, of degree q, say, then $b'_\mu = 0$, $c'_\mu = 0$, $b''_\mu = 0$ for $\mu \geqslant q + 2$.

For $\varepsilon = \frac{1}{2}$ and s not an integer it can be shown that $a'_\mu = 0$, $\mu = 1, 3, 5, \ldots$, in (3.2).

For $\varepsilon = 1$, if we replace $Q_h[f]$ in (3.1) by

$$\bar{Q}_h[f] = h^2 \sum_{i=1}^{n-1} w(ih) \sum_{j=0}^{n-i}{}'' f(ih, jh), \tag{3.4}$$

then for s not an integer

$$\bar{A}_h[f] = Q[f] - \bar{Q}_h[f] \sim \sum_{\mu=1}^{\infty} \bar{a}'_{2\mu} h^{2\mu} + \log h \sum_{\mu=0}^{\infty} \bar{b}'_\mu h^{\mu+s+1}$$
$$+ \sum_{\mu=0}^{\infty} \bar{c}'_\mu h^{\mu+s+1} \qquad \text{as} \quad h \to 0+. \tag{3.5}$$

4. Extensions to Arbitrary Simplices

So far we have considered the Euler–Maclaurin expansions for the standard simplex T. The results of Sections 2 and 3 can be extended to integrals of the form

$$\bar{Q}[g] = \iint_{\bar{T}} \tau(\xi, \eta)\, g(\xi, \eta)\, d\xi\, d\eta, \tag{4.1}$$

where $\bar{T}$ is the triangle with vertices $P_i = (\xi_i, \eta_i)$, $i = 1, 2, 3$, and $\tau(\xi, \eta) = |A\xi + B\eta + C|^s \quad (\log|A\xi + B\eta + C|)^{s'}$, $s > -1$, $s' = 0, 1$, such that $A\xi + B\eta + C = 0$ is the equation of the straight line joining P_1 and P_2, and $g(\xi, \eta)$ is infinitely differentiable over $\bar{T}$. Using a transformation of the form $\vec{\xi} = U\vec{x} + \vec{b}$, where $\vec{\xi} = \binom{\xi}{\eta}$, $\vec{x} = \binom{x}{y}$, and $\vec{b} = \binom{b_1}{b_2}$, and U is a 2×2 constant matrix, $\bar{T}$ can be mapped onto T with $P_1 \to (0, 0)$ and $P_2 \to (0, 1)$. The results of Sections 2 and 3 can now be applied to the transformed integral.

Bearing the results of the previous paragraph in mind, Euler–Maclaurin expansions can be derived for an arbitrary quadrilateral domain along one of whose diagonals the integrand has algebraic and/or logarithmic singularities.

This can be accomplished by treating the two triangles on both sides of the diagonal of singularities separately. One such typical integral is $\int_0^1 \int_0^1 |x-y|^s (\log|x-y|)^{s'} g(x,y)\,dx\,dy$, where $s > -1$, $s' = 0, 1$, which was the problem originally solved by the author (see Sidi [7]).

5. Euler–Maclaurin Expansions for $Q'[f]$

In this section we state the Euler–Maclaurin expansions to the integral $Q'[f]$.

THEOREM 5.1. *Let $f(x,y)$ be infinitely differentiable on Γ. Let ε and η be two fixed constants such that $0 \leqslant \varepsilon \leqslant 1$, $0 < \eta \leqslant 1$. Let $h = 1/n$, where n is a positive integer. Define*

$$Q'_h[f] = h^2 \sum_{i=0}^{n-1} w(ih+\eta h) \sum_{j=0}^{n-1} f(ih+\eta h, jh+\varepsilon h). \tag{5.1}$$

(1) *For $s' = 0$,*

$$\Delta'_h[f] \sim \sum_{\mu=1}^{\infty} A_\mu h^\mu + \sum_{\mu=0}^{\infty} B_\mu h^{\mu+s+1} \quad \text{as} \quad h \to 0+. \tag{5.2}$$

(2) *For $s' = 1$,*

$$\Delta'_h[f] \sim \sum_{\mu=1}^{\infty} A'_\mu h^\mu + \log h \sum_{\mu=0}^{\infty} B'_\mu h^{\mu+s+1} + \sum_{\mu=0}^{\infty} C'_\mu h^{\mu+s+1} \quad \text{as} \quad h \to 0+. \tag{5.3}$$

(3) *For $s' = 1$, $s = 0$,*

$$\Delta'_h[f] \sim \sum_{\mu=1}^{\infty} A''_\mu h^\mu + \log h \sum_{\mu=0}^{\infty} B''_\mu h^{\mu+1} \quad \text{as} \quad h \to 0+, \tag{5.4}$$

where A_μ, B_μ,..., are all independent of h and depend solely on $f(x,y)$ and its derivatives and their integrals.

Proof. Since the proofs of (5.2), (5.3), and (5.4) are very similar to those of Theorems 2.1, 3.1, and 3.2, respectively, we shall be content with a sketch of the proof of (5.2) only. Defining

$$F(x) = \int_0^1 f(x,y)\,dy, \tag{5.5}$$

we can express $Q'[f]$ as

$$Q'[f] = \int_0^1 x^s F(x)\,dx. \tag{5.6}$$

By Theorem 1.2 we have for any positive integer m

$$\begin{aligned} Q'[f] = h &\sum_{i=0}^{n-1} x^s F(x)|_{x=ih+\eta h} \\ &- \sum_{k=1}^{2m-1} \frac{B_k(\eta)}{k!} ([x^s F(x)]^{(k-1)}|_{x=1})\, h^k \\ &- \sum_{k=0}^{2m-1} \frac{\zeta(-s-k,\eta)}{k!} F^{(k)}(0)\, h^{k+s+1} + O(h^{2m}) \qquad \text{as} \quad h \to 0+. \end{aligned} \tag{5.7}$$

We now approximate $F(ih+\eta h)$ by the generalized trapezoidal rule. From Theorem 1.1 we have

$$\begin{aligned} F(ih+\eta h) = h &\sum_{j=0}^{n-1} f(ih+\eta h, jh+\varepsilon h) \\ &- \sum_{\mu=1}^{2m-1} \frac{B_\mu(\varepsilon)}{\mu!} \psi_{\mu-1}(ih+\eta h)\, h^\mu + \tau_{2m,i}, \end{aligned} \tag{5.8}$$

where

$$\psi_p(x) = \frac{\partial^p}{\partial y^p} f(x,y)|_{y=1} - \frac{\partial^p}{\partial y^p} f(x,y)|_{y=0}, \qquad p = 0, 1, \ldots, \tag{5.9}$$

and

$$|\tau_{2m,i}| \leqslant M_{2m} \max_{(x,y)\in T'} \left| \frac{\partial^{2m}}{\partial y^{2m}} f(x,y) \right| h^{2m}. \tag{5.10}$$

From here on the proof continues exactly as that of Theorem 2.1. In summary, defining $\theta_p^{(j)}(x)$ as in Section 2 (with $F(x)$, $\psi_p(x)$ as defined in (5.5) and (5.9)) we obtain

$$\begin{aligned} A_k &= -\sum_{\substack{\mu+\nu=k \\ \mu,\nu\geqslant 0}} \frac{B_\mu(\varepsilon)}{\mu!} \frac{B_\nu(\eta)}{\nu!} \theta^{(\nu)}_{\mu-1}(1), \qquad k = 1, 2, \ldots, \\ B_k &= -\sum_{\substack{\mu+\nu=k \\ \mu,\nu\geqslant 0}} \frac{B_\mu(\varepsilon)}{\mu!} \frac{\zeta(-s-\nu,\eta)}{\nu!} \psi^{(\nu)}_{\mu-1}(0), \qquad k = 0, 1, \ldots \end{aligned} \tag{5.11}$$ ∎

When $f(x, y)$ is a polynomial in x and y of degree q, say, then $B_k = 0$ for $k \geqslant q+2$.

If we let $\varepsilon = \eta = \frac{1}{2}$, then $A_k = 0$, $k = 1, 3, 5, \ldots$.

If we let (a) $\varepsilon = \eta = 1$, or (b) $\varepsilon = \frac{1}{2}$ and $\eta = 1$, or (c) $\varepsilon = 1$ and $\eta = \frac{1}{2}$, then none of the A_k's vanish in general. However, if $Q'_h[f]$ in (5.1) is modified to read, respectively,

$$\bar{Q}'_h[f] = h^2 \sum_{i=1}^{n}{}' w(ih) \sum_{j=0}^{n}{}'' f(ih, jh), \tag{5.12a}$$

$$\bar{Q}'_h[f] = h^2 \sum_{i=1}^{n}{}' w(ih) \sum_{j=0}^{n-1} f(ih, jh + h/2), \tag{5.12b}$$

or

$$\bar{Q}'_h[f] = h^2 \sum_{i=0}^{n-1} w(ih + h/2) \sum_{j=0}^{n}{}'' f(ih + h/2, jh), \tag{5.12c}$$

where $\sum_{i=1}^{\prime N} \alpha_i = \sum_{i=1}^{N-1} \alpha_i + \alpha_N/2$, then, using the same techniques as before, it can be shown that

$$\begin{aligned} \bar{A}'_h[f] &= Q'[f] - \bar{Q}'_h[f] \\ &= \sum_{\mu=1}^{\infty} \bar{A}_{2\mu} h^{2\mu} + \sum_{\mu=0}^{\infty} \bar{B}_\mu h^{\mu+s+1} \qquad \text{as} \quad h \to 0+. \end{aligned} \tag{5.13}$$

Similar analysis can be done for $s' = 1$ also. Details will not be given here.

6. Concluding Remarks

In this work Euler–Maclaurin expansions for the integrals given in (1.1)–(1.2) were derived and their nature was analyzed. These expansions can now be used to obtain good approximations to the integrals in question by applying to them a generalization of the Richardson extrapolation process (see Sidi [6]). A detailed discussion about how this should be done and some numerical examples can be found in Sidi [7].

Euler–Maclaurin expansions for singular multiple integrals over a hypercube have been taken up by Lyness [1], where the integrand is assumed to have a singularity at a *corner* of the hypercube. Lately, Monegato and Lyness [3] have considered the question of numerically evaluating the Cauchy principal value of integrals of the form $\int_0^1 \int_0^1 g(x, y)/(x - y)\, dx\, dy$. More recently Lyness and Monegato [2] have given Euler–Maclaurin expansions for integrals over the hypersimplex, whose integrands have singularities at the vertices of the hypersimplex. The integrals treated in this work, however, are not of either type; they have algebraic and/or logarithmic singularities over a straight line inside or on the boundary of the domain of integration.

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