



Numerical integration over smooth surfaces in \mathbb{R}^3 via class \mathcal{S}_m variable transformations. Part I: Smooth integrands

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Abstract

Class \mathcal{S}_m variable transformations with integer m for finite-range integrals were introduced by the author about a decade ago. These transformations “periodize” the integrand functions in a way that enables the trapezoidal rule to achieve very high accuracy, especially with even m . In a recent work by the author, these transformations were extended to *arbitrary* real m , and their role in improving the convergence of the trapezoidal rule for different classes of integrands was studied in detail. It was shown that, with m chosen appropriately, exceptionally high accuracy can be achieved by the trapezoidal rule. For example, if the integrand function is smooth on the interval of integration including the endpoints, and vanishes at the endpoints, then excellent results are obtained by taking $2m$ to be an odd integer. In the present work, we consider the use of these transformations in the computation of integrals on surfaces of simply connected bounded domains in \mathbb{R}^3 , in conjunction with the product trapezoidal rule. We assume these surfaces are smooth and homeomorphic to the surface of the unit sphere, and we treat the cases in which the integrands are smooth. We propose two approaches, one in which the product trapezoidal rule is applied with the integrand as is, and another, in which the integrand is preprocessed before the rule is applied. We give thorough analyses of the errors incurred in both approaches, which show that surprisingly

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high accuracies can be achieved with suitable values of m . We also illustrate the theoretical results with numerical examples.

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1. Introduction

In this work, we present a new approach to the numerical evaluation of integrals over smooth surfaces in three dimensions. We treat integrals of the form

$$I[f] = \int_S f(Q) dA_S, \quad (1.1)$$

where S is the surface of an arbitrary bounded and simply connected domain in \mathbb{R}^3 and dA_S is the associated area element. We assume that S is infinitely smooth and homeomorphic to the surface of the unit sphere, which we shall denote by U throughout. We also assume that the transformation from U to S is one-to-one and infinitely differentiable and that it has a nonsingular Jacobian matrix.

The integrand functions $f(Q)$ we consider are smooth over S . (In another work [19], we treat the cases in which the integrand functions have point singularities of the single-layer and double-layer types over S .)

Such integrals, with smooth or singular $f(Q)$, arise in boundary integral equation formulations of partial differential equations in continuum problems. For a review of this subject, see Atkinson [2] and [3, Chapter 5].

Here are the steps of the basic method of integration we present in this work:

- (i) Using the mapping of U , the surface of the unit sphere, to S , express $I[f]$ as an integral over U .
- (ii) Express the (transformed) integral over U in terms of the standard spherical coordinates θ and ϕ , $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$. The resulting integral can be written in the form $I[f] = \int_0^\pi \left[\int_0^{2\pi} F(\theta, \phi) d\phi \right] d\theta$.
- (iii) Transform θ by a variable transformation $\theta = \Psi(t) \equiv \pi\psi(t)$, $0 \leq t \leq 1$, where $\psi(t)$ is in the extended class \mathcal{S}_m of Sidi [22]. The result of this is $I[f] = \int_0^1 \left[\int_0^{2\pi} F(\Psi(t), \phi) d\phi \right] \Psi'(t) dt$.
- (iv) Approximate the final integral in the variables t and ϕ by the product trapezoidal rule.

Note. The basic method above, although quite effective as is, can be improved substantially by applying it to $I[f - r]$ for some suitably (and simply) chosen function $r(Q)$, such that $I[r]$ is much less expensive to compute than $I[f]$. We will discuss the details of this improved procedure later.

The complete mathematical description of the basic method is given in the next paragraph.

Let $Q = (\xi, \eta, \zeta)$ in (1.1), and let U , the surface of the unit sphere, be given as in

$$U := \{(x, y, z) : x^2 + y^2 + z^2 = 1\}. \tag{1.2}$$

Denote the mapping from U to S via

$$\boldsymbol{\rho} = [\xi, \eta, \zeta]^T = [\xi(x, y, z), \eta(x, y, z), \zeta(x, y, z)]^T, \tag{1.3}$$

so that the Jacobian matrix of this mapping is

$$J(x, y, z) = \begin{bmatrix} \partial\xi/\partial x & \partial\xi/\partial y & \partial\xi/\partial z \\ \partial\eta/\partial x & \partial\eta/\partial y & \partial\eta/\partial z \\ \partial\zeta/\partial x & \partial\zeta/\partial y & \partial\zeta/\partial z \end{bmatrix}. \tag{1.4}$$

Thus, $J(x, y, z)$ is known as a function of x, y, z . We also let

$$\mathbf{r} = [x, y, z]^T, \tag{1.5}$$

and then switch to the spherical coordinates θ and ϕ as in

$$(x, y, z) = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta). \tag{1.6}$$

Now, by expressing $I[f]$ as an integral over U via (1.3), and by introducing the variables θ and ϕ on U as in (1.6), we are actually generating a two-parameter representation of S , these parameters being θ and ϕ . Thus, in terms of θ and ϕ , the area element dA_S on S becomes

$$dA_S = \left\| \frac{\partial \boldsymbol{\rho}}{\partial \theta} \times \frac{\partial \boldsymbol{\rho}}{\partial \phi} \right\| d\theta d\phi, \tag{1.7}$$

where $\|\mathbf{p}\| = \sqrt{\mathbf{p}^T \mathbf{p}}$ for $\mathbf{p} \in \mathbb{R}^3$. We, therefore, have

$$I[f] = \int_0^\pi \left[\int_0^{2\pi} F(\theta, \phi) d\phi \right] d\theta; \quad F(\theta, \phi) \equiv f(\xi, \eta, \zeta) \left\| \frac{\partial \boldsymbol{\rho}}{\partial \theta} \times \frac{\partial \boldsymbol{\rho}}{\partial \phi} \right\|. \tag{1.8}$$

The vectors $\partial \boldsymbol{\rho} / \partial \theta$ and $\partial \boldsymbol{\rho} / \partial \phi$ can be computed by the chain rule, as in

$$\frac{\partial \boldsymbol{\rho}}{\partial \theta} = J \frac{\partial \mathbf{r}}{\partial \theta}, \quad \frac{\partial \boldsymbol{\rho}}{\partial \phi} = J \frac{\partial \mathbf{r}}{\partial \phi}. \tag{1.9}$$

Here, J stands for $J(x, y, z)$ for short, and

$$\frac{\partial \mathbf{r}}{\partial \theta} = \begin{bmatrix} \cos \theta \cos \phi \\ \cos \theta \sin \phi \\ -\sin \theta \end{bmatrix}, \quad \frac{\partial \mathbf{r}}{\partial \phi} = \sin \theta \begin{bmatrix} -\sin \phi \\ \cos \phi \\ 0 \end{bmatrix}. \tag{1.10}$$

Finally, we make the further variable transformation $\theta = \Psi(t) = \pi\psi(t)$, with $\psi \in \mathcal{S}_m$ for some suitable m to be chosen later, obtaining

$$I[f] = \int_0^1 \left[\int_0^{2\pi} \widehat{F}(t, \phi) d\phi \right] dt; \quad \widehat{F}(t, \phi) = F(\Psi(t), \phi)\Psi'(t), \tag{1.11}$$

and approximate the transformed integral via the product trapezoidal rule

$$\widehat{T}_{n,n'}[f] = hh' \sum_{j=1}^{n-1} \sum_{k=1}^{n'} \widehat{F}(jh, kh'); \quad h = \frac{1}{n}, \quad h' = \frac{2\pi}{n'}, \tag{1.12}$$

where n and n' are positive integers. We let $n' \sim \alpha n$ as $n \rightarrow \infty$ for some fixed α in the sequel.

Note that the product trapezoidal rule for an arbitrary integral $\int_0^1 \left[\int_0^{2\pi} \widehat{F}(t, \phi) d\phi \right] dt$, where \widehat{F} is continuous for $(t, \phi) \in [0, 1] \times [0, 2\pi]$, is actually $hh' \sum_{j=0}^{n-1} \sum_{k=0}^{n'} \widehat{F}(jh, kh')$, where the double prime on a summation means that the first and the last terms in the summation are to be multiplied by 1/2. $\widehat{T}_{n,n'}[f]$ in (1.12) becomes the product trapezoidal rule in case $\widehat{F}(0, \phi) = 0 = \widehat{F}(1, \phi)$ and $\widehat{F}(t, \phi)$ is 2π -periodic in ϕ , which is the case we have here starting with $m = 1$.

The variable transformation $\theta = \Psi(t)$ above turns out to be very effective in that the accuracy of $\widehat{T}_{n,n'}[f]$ increases with increasing m , and in a subtle way. For odd integer values of $2m$, unusually high accuracies are achieved, as we will see later.

The plan of this paper is as follows: In the remainder of this section, we discuss briefly the subject of variable transformations in numerical integration. In Section 2, we derive the form of the integral that is obtained following the various mappings. Following that, in Section 3, we give a complete asymptotic analysis as $h \rightarrow 0$ of the product rule $\widehat{T}_{n,n'}[f]$. The main result of this section is Theorem 3.3. In Section 4, we give an improved approach to the computation of $I[f]$. In this approach, the integrand is preprocessed by subtracting from it a suitably chosen function, as mentioned in the note above, and the product rule is applied to this modified integrand. The main result of Section 4 is Theorem 4.2. We also provide numerical examples with both approaches, and verify the validity of our theoretical results.

For easy reference, we have also included three appendices that provide a short discussion, based on the paper [22], of the Euler–Maclaurin expansions relevant to this work and of the extended class \mathcal{S}_m . Of these, [Appendix A](#) gives

the Euler–Maclaurin expansions. Appendix B describes the extended class \mathcal{S}_m generally and gives the extended \sin^m -transformation, a representative of the extended class \mathcal{S}_m , which we have used in our computations. Appendix C summarizes the analytic properties of transformations in the extended class \mathcal{S}_m that pertain to the present work.

Before closing, we mention that the basic method described above is related to a recent method of Atkinson [4]. As it turns out, the numerical performance of our basic method is very similar to that of [4], and some of the theoretical results of Section 3 concerning our basic method are analogous to those of [4]. There is no analogue of our improved method and its corresponding theory in [4], however. One of the major differences between the methods of the present paper and that of [4] is that in the present paper, the variable θ on the unit sphere is transformed (by a variable transformation in the extended class \mathcal{S}_m), whereas in [4], θ is “graded” in a special and interesting way by the introduction of a grading parameter, instead of being transformed.

Finally, this paper is partly based on the report [18] by the author.

1.1. Variable transformations in numerical integration

In order to have a better understanding of the methods presented in this work, it is necessary to dwell briefly on the subject of variable transformations in numerical integration.

Consider the integral

$$I[f] = \int_0^1 f(x) dx, \quad (1.13)$$

where $f \in C^\infty(0, 1)$ but is not necessarily continuous or differentiable at $x = 0$ and/or $x = 1$. $f(x)$ may even behave singularly at the endpoints, with different types of singularities. One very effective way of computing $I[f]$ is by first transforming it with a suitable variable transformation and next applying the trapezoidal rule to the resulting transformed integral. Thus, if we make the substitution $x = \psi(t)$, where $\psi(t)$ is an increasing differentiable function on $[0, 1]$, such that $\psi(0) = 0$ and $\psi(1) = 1$, then the transformed integral is

$$I[f] = \int_0^1 \hat{f}(t) dt; \quad \hat{f}(t) = u(\psi(t))\psi'(t), \quad (1.14)$$

and the trapezoidal rule approximation to $I[f]$ is

$$\widehat{Q}_n[f] = h \left[\frac{1}{2} \hat{f}(0) + \sum_{i=1}^{n-1} \hat{f}(ih) + \frac{1}{2} \hat{f}(1) \right]; \quad h = \frac{1}{n}. \quad (1.15)$$

If, in addition, $\psi(t)$ is chosen such that $\psi^{(i)}(0) = \psi^{(i)}(1) = 0$, $i = 1, 2, \dots, p$, for some sufficiently large p , then $\widehat{Q}_n[f]$, even for moderate n , approximate $I[f]$ with surprisingly high accuracy. In such a case, we may have $f(0) = \hat{f}(1) = 0$, and $\widehat{Q}_n[f]$ becomes

$$\widehat{Q}_n[f] = h \sum_{i=1}^{n-1} \widehat{f}(ih). \tag{1.16}$$

Variable transformations in numerical integration have been of considerable interest lately. In the context of one-dimensional integration, they are used as a means to improve the performance of the trapezoidal rule. In the context of multi-dimensional integration, they are used to “periodize” the integrand in all variables so as to improve the accuracy of lattice rules. (Lattice rules are extensions of the trapezoidal rule to many dimensions.)

There is a whole collection of variable transformations in the literature of numerical integration. We mention here the polynomial transformation of Korobov [9], the tanh-transformation of Sag and Szekeres [15], the IMT-transformation of Iri, Moriguti, and Takasawa [8], the double exponential formula of Mori [12], the class \mathcal{S}_m transformations (m is a positive integer) of Sidi [17], and the polynomial transformation of Laurie [10].

In this paper, we concentrate on the class \mathcal{S}_m transformations of the author, which have some interesting and useful properties when coupled with the trapezoidal rule. A trigonometric representative of these, namely, the \sin^m -transformation that was proposed also in [17], has been used successfully in conjunction with lattice rules in multiple integration; see Sloan and Joe [23], Hill and Robinson [7], and Robinson and Hill [14]. The \sin^m -transformation has also been used in the computation of multidimensional integrals in conjunction with extrapolation methods by Verlinden et al. [24].

Another trigonometric transformation similar to the \sin^m -transformation was given by Elliott [6], and this transformation too is in the class \mathcal{S}_m with even m . The polynomial transformation of Laurie was designed to have some of the useful properties of class \mathcal{S}_m transformations, but is not in \mathcal{S}_m .

Recently, the class \mathcal{S}_m was extended to arbitrary *noninteger* values of m in Sidi [22]. Transformations in this extended class were analyzed with respect to their use in conjunction with the trapezoidal rule, and were shown to improve the accuracy of the resulting approximations beyond what is expected, when m is chosen *optimally*.

2. The transformed integrand

In this section, we wish to carry out a preliminary study of the integrand $F(\theta, \phi)$ in (1.8). As we already know the nature of $f(\xi, \eta, \zeta)$, we concentrate on the factor $\|\partial \boldsymbol{\rho} / \partial \theta \times \partial \boldsymbol{\rho} / \partial \phi\|$ in (1.8). For simplicity of notation, we will denote (ξ, η, ζ) by (ξ_1, ξ_2, ξ_3) and (x, y, z) by (x_1, x_2, x_3) . Similarly, we denote the mapping from U to S via

$$\boldsymbol{\rho} = [\xi_1(x_1, x_2, x_3), \xi_2(x_1, x_2, x_3), \xi_3(x_1, x_2, x_3)]^T, \tag{2.1}$$

and let

$$\mathbf{r} = [x_1, x_2, x_3]^T, \tag{2.2}$$

so that, in the spherical coordinates θ and ϕ ,

$$(x_1, x_2, x_3) = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta). \tag{2.3}$$

Denoting

$$\begin{bmatrix} \cos \theta \cos \phi \\ \cos \theta \sin \phi \\ -\sin \theta \end{bmatrix} = \boldsymbol{\kappa}, \quad \begin{bmatrix} -\sin \phi \\ \cos \phi \\ 0 \end{bmatrix} = \boldsymbol{\lambda} \tag{2.4}$$

in (1.10), and also letting

$$\mathbf{K} = J\boldsymbol{\kappa}, \quad \mathbf{L} = J\boldsymbol{\lambda}, \tag{2.5}$$

(1.9) becomes

$$\frac{\partial \boldsymbol{\rho}}{\partial \theta} = \mathbf{K}, \quad \frac{\partial \boldsymbol{\rho}}{\partial \phi} = \mathbf{L} \sin \theta, \tag{2.6}$$

and we have

$$\frac{\partial \boldsymbol{\rho}}{\partial \theta} \times \frac{\partial \boldsymbol{\rho}}{\partial \phi} = \mathbf{M} \sin \theta; \quad \mathbf{M} = \mathbf{K} \times \mathbf{L}. \tag{2.7}$$

Letting also $\mathbf{K} = [K_1, K_2, K_3]^T$ and $\mathbf{L} = [L_1, L_2, L_3]^T$, we have

$$\mathbf{M} = [\sigma_{23}, \sigma_{31}, \sigma_{12}]^T; \quad \sigma_{ij} = K_i L_j - K_j L_i. \tag{2.8}$$

Now, by (2.5), there follows

$$\sigma_{ij} = \sum_{r=1}^3 \sum_{s=1}^3 J_{ir} J_{js} \tau_{rs}; \quad \tau_{rs} = \kappa_r \lambda_s - \kappa_s \lambda_r. \tag{2.9}$$

Here J_{ij} is the (i, j) element of the matrix J .

Obviously, $\tau_{sr} = -\tau_{rs}$ and $\tau_{rr} = 0$. This means that there are really three independent τ_{rs} , namely, τ_{12} , τ_{23} , and τ_{31} . By (2.4), these are

$$\tau_{12} = \cos \theta = x_3, \quad \tau_{23} = \sin \theta \cos \phi = x_1, \quad \tau_{31} = \sin \theta \sin \phi = x_2.$$

Thus, we can express τ_{ij} , for all i and j , as in

$$\tau_{ij} = \sum_{k=1}^3 \epsilon_{ijk} x_k,$$

where $\epsilon_{123} = 1$, and ϵ_{ijk} , $1 \leq i, j, k \leq 3$, is odd under an interchange of any two of the indices i, j, k , which means that $\epsilon_{ijk} = 0$ when any two of these indices have the same value. Substituting these in (2.9), and invoking $J_{ij} = \partial \xi_j / \partial x_i$, we obtain

$$\sigma_{ij} = \sum_{r=1}^3 \sum_{s=1}^3 \sum_{k=1}^3 \epsilon_{rsk} \frac{\partial \xi_i}{\partial x_r} \frac{\partial \xi_j}{\partial x_s} x_k = (\nabla \xi_i \times \nabla \xi_j) \cdot \mathbf{r}. \tag{2.10}$$

Here, ∇u is the gradient of $u(x, y, z)$, that is, $\nabla u = (\partial u/\partial x, \partial u/\partial y, \partial u/\partial z)$.

First, we note by (2.10) that σ_{ij} , as functions of (x_1, x_2, x_3) , are all in $C^\infty(U)$ because $\partial \xi_i/\partial x_j \in C^\infty(U)$ by the assumptions we have made on the mapping from U to S .

Next, we wish to show that σ_{12} , σ_{23} , and σ_{31} cannot vanish simultaneously at any point on U . An important implication of this for us is that $M(x, y, z) = \sigma_{23}^2 + \sigma_{31}^2 + \sigma_{12}^2$ is strictly positive on U , as a result which, $\sqrt{M(x, y, z)}$ is in $C^\infty(U)$. Suppose, to the contrary, that at some point $(a, b, c) \in U$, $\sigma_{12} = \sigma_{23} = \sigma_{31} = 0$. This means that all three vectors $\nabla \xi_i(a, b, c)$, $i = 1, 2, 3$, lie in a plane orthogonal to the vector $[a, b, c]^T$, hence lie in the same plane, thus becoming linearly dependent. This is equivalent to $\det J(a, b, c) = 0$, which contradicts our assumption that the matrix $J(x, y, z)$ is nonsingular on U .

We have thus proved the following result:

Theorem 2.1. *With S as in the first paragraph of Section 1, there holds*

$$\frac{\partial \rho}{\partial \theta} \times \frac{\partial \rho}{\partial \phi} = [\sigma_{23}, \sigma_{31}, \sigma_{12}]^T \sin \theta, \quad \left\| \frac{\partial \rho}{\partial \theta} \times \frac{\partial \rho}{\partial \phi} \right\| = R(x, y, z) \sin \theta, \tag{2.11}$$

where

$$R(x, y, z) = \sqrt{\sigma_{23}^2 + \sigma_{31}^2 + \sigma_{12}^2}; \quad \sigma_{ij} = (\nabla \xi_i \times \nabla \xi_j) \cdot \mathbf{r}. \tag{2.12}$$

$R(x, y, z)$ is strictly positive on U and is in $C^\infty(U)$. Consequently, $R(x, y, z)$, as a function of ϕ , is infinitely differentiable on $(-\infty, \infty)$ and 2π -periodic as well.

Note that the result of Theorem 2.1 is true whether S has symmetry properties or not.

As an example, let us consider the case in which S is the surface of an ellipsoid, which we take to be

$$S = \left\{ (\xi, \eta, \zeta) : (\xi/a)^2 + (\eta/b)^2 + (\zeta/c)^2 = 1 \right\}. \tag{2.13}$$

Here, a, b, c are the lengths of the semi-axes of this ellipsoid. The mapping from U to S can be taken to be $(\xi, \eta, \zeta) = (ax, by, cz)$. In this case, $J = \text{diag}(a, b, c)$ hence is nonsingular on U . This example was treated in [4], where the result

$$R(x, y, z) = \left[(bcx)^2 + (cay)^2 + (abz)^2 \right]^{1/2}, \tag{2.14}$$

is also given. This result can also be obtained from Theorem 2.1. It is easy to see that $R(x, y, z)$ in this case is in $C^\infty(U)$, and this is in accordance with Theorem 2.1.

3. Study of $\widehat{T}_{n,n'}[f]$ for smooth $f(Q)$

Let us combine (2.11) and (1.8), and rewrite the latter in the form

$$I[f] = \int_0^\pi \left[\int_0^{2\pi} F(\theta, \phi) \, d\phi \right] d\theta = \int_0^\pi v(\theta) \, d\theta;$$

$$v(\theta) = \int_0^{2\pi} F(\theta, \phi) \, d\phi, \quad F(\theta, \phi) = w(x, y, z) \sin \theta,$$

$$w(x, y, z) = f(\zeta, \eta, \zeta)R(x, y, z).$$

Transforming the variable θ via $\theta = \Psi(t)$, where $\Psi(t) = \pi\psi(t)$ with $\psi \in \mathcal{S}_m$ for some m , we also have

$$I[f] = \int_0^1 \left[\int_0^{2\pi} \widehat{F}(t, \phi) \, d\phi \right] dt = \int_0^1 \widehat{v}(t) \, dt;$$

$$\widehat{v}(t) = \int_0^{2\pi} \widehat{F}(t, \phi) \, d\phi, \quad \widehat{F}(t, \phi) = F(\Psi(t), \phi)\Psi'(t),$$

$$\widehat{v}(t) = v(\Psi(t))\Psi'(t).$$

By our assumptions that (i) $f(\zeta, \eta, \zeta)$ is infinitely differentiable over S and (ii) the mapping from U to S is infinitely differentiable on U , we have that $f(\zeta, \eta, \zeta)$ is infinitely differentiable over U as a function of (x, y, z) . From Theorem 2.1, we also have that $R(x, y, z)$ is infinitely differentiable on U . Consequently, $w(x, y, z)$ is infinitely differentiable on U . Therefore, as a function of the variable ϕ , $F(\theta, \phi)$ is infinitely differentiable on $(-\infty, \infty)$ and also 2π -periodic. Therefore, $\widehat{F}(t, \phi)$, as a function ϕ , is also infinitely differentiable on $(-\infty, \infty)$ and is also 2π -periodic.

Let us rewrite (1.12) in the form

$$\widehat{T}_{n,n'}[f] = h \sum_{j=1}^{n-1} \left[h' \sum_{k=1}^{n'} \widehat{F}(jh, kh') \right]; \quad h = \frac{1}{n}, \quad h' = \frac{2\pi}{n'}.$$

Now, $h' \sum_{k=1}^{n'} \widehat{F}(t, kh')$ is the trapezoidal rule approximation to the integral $\int_0^{2\pi} \widehat{F}(t, \phi) \, d\phi$. Therefore, by the Euler–Maclaurin summation formula in Theorem A.1, and by the fact that $\widehat{F}(t, \phi)$, as a function ϕ , is also infinitely differentiable on $(-\infty, \infty)$ and also 2π -periodic, we have

$$h' \sum_{k=1}^{n'} \widehat{F}(t, kh') = \int_0^{2\pi} \widehat{F}(t, \phi) \, d\phi + R_m(t; h'), \tag{3.1}$$

where

$$|R_m(t; h')| \leq 2\pi \frac{B_{2m}}{(2m)!} \left(\max_{\substack{0 \leq i \leq 1 \\ 0 \leq \phi \leq 2\pi}} \left| \frac{\partial^{2m}}{\partial \phi^{2m}} \widehat{F}(t, \phi) \right| \right) h^{2m} \\ \equiv C_m h^{2m} \quad \text{for every } m, \tag{3.2}$$

where C_m is a constant independent of t . Consequently,

$$\widehat{T}_{n,n'}[f] = \widetilde{T}_n[f] + O(h^\mu) \quad \text{as } h' \rightarrow 0, \text{ for every } \mu > 0. \tag{3.3}$$

where

$$\widetilde{T}_n[f] = h \sum_{j=1}^{n-1} \int_0^{2\pi} \widehat{F}(jh, \phi) d\phi = h \sum_{j=1}^{n-1} \widehat{v}(jh). \tag{3.4}$$

Thus, if we let $n' \sim \alpha n^\beta$ as $n \rightarrow \infty$ for some fixed positive α and β , then (3.4) becomes

$$\widehat{T}_{n,n'}[f] = \widetilde{T}_n[f] + O(h^\mu) \quad \text{as } h \rightarrow 0, \text{ for every } \mu > 0. \tag{3.5}$$

In the sequel, we let $n' \sim \alpha n^\beta$ as $n \rightarrow \infty$.

Thus, we need to concern ourselves only with the asymptotic expansion as $h \rightarrow 0$ of $\widetilde{T}_n[f]$, the trapezoidal rule approximation to the integral $\int_0^1 \widehat{v}(t) dt$. By Theorem A.2, we need to study $\widehat{v}(t)$ as $t \rightarrow 0+$ and $t \rightarrow 1-$. For this, we need to expand $\widehat{F}(t, \phi)$ about $t = 0$ and $t = 1$. This we do by expanding $v(\theta)$ about $\theta = 0$ and $\theta = \pi$, for which we need to expand $F(\theta, \phi)$ about $\theta = 0$ and $\theta = \pi$.

Throughout, we make use of the fact that the sequence $\{(\sin \theta)^i\}_{i=1}^\infty$ is a non-afide asymptotic scale both as $\theta \rightarrow 0$ and as $\theta \rightarrow \pi$.

Now, by (1.6), $x = y = 0$ and $z = 1$ when $\theta = 0$, and $x = y = 0$ and $z = -1$ when $\theta = \pi$. Therefore, $w(x, y, z)$ has the asymptotic expansions

$$w(x, y, z) \sim \sum_{i=0}^\infty \sum_{j=0}^\infty \sum_{k=0}^\infty \frac{w^{(i,j,k)}(0, 0, 1)}{i!j!k!} x^i y^j (z - 1)^k \quad \text{as } \theta \rightarrow 0,$$

$$w(x, y, z) \sim \sum_{i=0}^\infty \sum_{j=0}^\infty \sum_{k=0}^\infty \frac{w^{(i,j,k)}(0, 0, -1)}{i!j!k!} x^i y^j (z + 1)^k \quad \text{as } \theta \rightarrow \pi,$$

where

$$w^{(i,j,k)}(x_0, y_0, z_0) = \left. \frac{\partial^{i+j+k} w}{\partial x^i \partial y^j \partial z^k} \right|_{(x,y,z)=(x_0,y_0,z_0)}.$$

These are simply the Taylor series expansions of $w(x, y, z)$ about $(0, 0, \pm 1)$. Using the short-hand notation $\sum_{i,j,k \geq 0} = \sum_{i=0}^\infty \sum_{j=0}^\infty \sum_{k=0}^\infty$, and invoking (1.6), these expansions can be rewritten in the form

$$w(x, y, z) \sim \sum_{i,j,k \geq 0} e_{i,j,k}^{(+)} \cos^i \phi \sin^j \phi (\sin \theta)^{i+j} (\cos \theta - 1)^k \quad \text{as } \theta \rightarrow 0,$$

$$w(x, y, z) \sim \sum_{i,j,k \geq 0} e_{i,j,k}^{(-)} \cos^i \phi \sin^j \phi (\sin \theta)^{i+j} (\cos \theta + 1)^k \quad \text{as } \theta \rightarrow \pi,$$

where

$$e_{i,j,k}^{(\pm)} = \frac{w^{(i,j,k)}(0, 0, \pm 1)}{i!j!k!}.$$

Therefore,

$$\begin{aligned} F(\theta, \phi) &\sim \sum_{i,j,k \geq 0} e_{i,j,k}^{(+)} \cos^i \phi \sin^j \phi (\sin \theta)^{i+j+1} (\cos \theta - 1)^k \quad \text{as } \theta \rightarrow 0, \\ F(\theta, \phi) &\sim \sum_{i,j,k \geq 0} e_{i,j,k}^{(-)} \cos^i \phi \sin^j \phi (\sin \theta)^{i+j+1} (\cos \theta + 1)^k \quad \text{as } \theta \rightarrow \pi. \end{aligned} \tag{3.6}$$

The following general lemma will be of use in the sequel.

Lemma 3.1. *Let $M(\phi)$ be an even and π -periodic function of ϕ . Define $u(\phi) = M(\phi) \cos^i \phi \sin^j \phi$ and $q_{i,j} = \int_0^{2\pi} u(\phi) d\phi$. If i or j or both are odd integers, then $q_{i,j} = 0$. Thus, $q_{i,j}$ is possibly nonzero only if i and j are both even integers.*

Proof. First, note that, because $u(\phi)$ is 2π -periodic, we have that $q \equiv q_{i,j} = \int_{-\pi}^{\pi} u(\phi) d\phi$. With μ and ν nonnegative integers, there are three cases to consider: (a) $i = 2\mu + 1$ and $j = 2\nu + 1$, (b) $i = 2\mu$ and $j = 2\nu + 1$, and (c) $i = 2\mu + 1$ and $j = 2\nu$. Let us also denote $K(\phi) = M(\phi) \cos^{2\mu} \phi \sin^{2\nu} \phi$. Obviously, $K(\phi)$ is also an even and π -periodic function of ϕ .

In case (a), $u(\phi) = K(\phi) \cos \phi \sin \phi = \frac{1}{2}K(\phi) \sin 2\phi$, and is an odd function. Therefore, $q = 0$. In case (b), $u(\phi) = K(\phi) \sin \phi$, and is an odd function. Therefore, $q = 0$. In case (c), $u(\phi) = K(\phi) \cos \phi$, and is an even function. Thus, $q = 2 \int_0^{\pi} K(\phi) \cos \phi$. By the fact that $K(\phi)$ is even and π -periodic, we can write this as $q = 2 \int_0^{\pi} K(\pi - \phi) \cos \phi$. Upon making the variable transformation $\phi = \pi - \omega$ in the last integral, we obtain $q = -2 \int_0^{\pi} K(\omega) \cos \omega d\omega = -q$. This implies $q = 0$. \square

Theorem 3.2. *When $f(\xi, \eta, \zeta)$ is smooth over S , $v(\theta) = \int_0^{2\pi} F(\theta, \phi) d\phi$ has the asymptotic expansions*

$$\begin{aligned} v(\theta) &\sim \sum_{i,j,k \geq 0} A_{i,j,k}^{(+)} (\sin \theta)^{2i+2j+1} (\cos \theta - 1)^k \quad \text{as } \theta \rightarrow 0, \\ v(\theta) &\sim \sum_{i,j,k \geq 0} A_{i,j,k}^{(-)} (\sin \theta)^{2i+2j+1} (\cos \theta + 1)^k \quad \text{as } \theta \rightarrow \pi, \end{aligned} \tag{3.7}$$

where $A_{i,j,k}^{(\pm)}$ are constants given by

$$A_{i,j,k}^{(\pm)} = e_{2i,2j,k}^{(\pm)} \int_0^{2\pi} (\cos \phi)^{2i} (\sin \phi)^{2j} d\phi, \quad i, j, k = 0, 1, \dots$$

Consequently,

$$\begin{aligned} v(\theta) &\sim \sum_{i=0}^{\infty} \mu_i^{(+)} \theta^{2i+1} \quad \text{as } \theta \rightarrow 0; \\ v(\theta) &\sim \sum_{i=0}^{\infty} \mu_i^{(-)} (\pi - \theta)^{2i+1} \quad \text{as } \theta \rightarrow \pi, \end{aligned} \tag{3.8}$$

for some constants $\mu_i^{(\pm)}$.

Proof. To prove the first part of the theorem, we substitute (3.6) in the integral $\int_0^{2\pi} F(\theta, \phi) d\phi$, interchange the order of integration and summation (which is allowed because the integration is over the finite interval $[0, 2\pi]$), and invoke Lemma 3.1. To prove the second part, we proceed as follows. Because

$$\begin{aligned} \sin \theta &= \sin(\pi - \theta), \quad \cos \theta - 1 = 2 \sin^2 \frac{\theta}{2}, \\ \cos \theta + 1 &= 2 \cos^2 \frac{\theta}{2} = \sin^2 \frac{\pi - \theta}{2}, \end{aligned}$$

it is clear that the asymptotic expansions of $v(\theta)$ as $\theta \rightarrow 0$ and as $\theta \rightarrow \pi$ contain only odd powers of θ and $(\pi - \theta)$, respectively. This proves the second part of the theorem. \square

Making now the variable transformation $\theta = \pi\psi(t)$ in $\int_0^\pi v(\theta) d\theta$, where $\psi \in \mathcal{S}_m$, and invoking first Theorem 3.2 and next part (i) of Theorem C.1 and part(iii) of Corollary C.2, we obtain the following main result. We leave the details of the proof to the reader.

Theorem 3.3. *With $\psi(t)$ in \mathcal{S}_m , and with $n' \sim \alpha n^\beta$ as $n \rightarrow \infty$ for some fixed positive α and β , there holds*

$$\widehat{T}_{n,n'}[f] - I[f] = \begin{cases} O(h^{4m+4}) & \text{as } h \rightarrow 0, \text{ if } 2m \text{ odd integer,} \\ O(h^{2m+2}) & \text{as } h \rightarrow 0, \text{ otherwise.} \end{cases}$$

For $2m$ an odd integer, we also have the complete Euler–Maclaurin expansion

$$\widehat{T}_{n,n'}[f] \sim I[f] + \sum_{i=0}^{\infty} \sigma_i h^{4m+4+2i} \quad \text{as } h \rightarrow 0.$$

For integer values of m , we have

$$\widehat{T}_{n,n'}[f] \sim I[f] + \sum_{i=0}^{\infty} \sigma_i h^{2m+2+2i} \quad \text{as } h \rightarrow 0.$$

For all other values of m , we have

$$\widehat{T}_{n,n'}[f] \sim I[f] + \sum_{\substack{k=1 \\ 2km \notin \{1,3,5,\dots\}}}^{\infty} \sum_{i=0}^{\infty} \sigma_{k,i} h^{2k(m+1)+2i} \quad \text{as } h \rightarrow 0.$$

Note the remarkable accuracy that $\widehat{T}_{n,n'}[f]$ can achieve when $2m$ is an odd integer. This is especially due to the fact that the asymptotic expansions of $v(\theta)$, as $\theta \rightarrow 0$ and $\theta \rightarrow \pi$, do not contain the powers θ^{2i} and $(\pi - \theta)^{2i}$, $i = 0, 1, \dots$, respectively.

3.1. A numerical example

Let S be the surface of the ellipsoid given in (2.13) with $(a, b, c) = (1.0, 0.5, 0.75)$, and let $f(Q) = f(\xi, \eta, \zeta) = \exp(\xi + 2\eta + 3\zeta)$, and consider the integral

$$I[f] = \int_S \int_S f(Q) dA_S = 18.34041919200 \dots$$

This is one of the numerical examples treated in [4].

The transformation we use for the variable θ is the \sin^m -transformation for various values of m . Clearly, the integrand $f(\xi, \eta, \zeta)$ is infinitely differentiable over S , hence Theorems 3.2 and 3.3 apply.

The numerical results in Tables 1 and 2, which were computed in quadruple-precision arithmetic, illustrate the result of Theorem 3.3 very clearly. Table 1 gives the relative errors in the $\widehat{T}_n[f] \equiv \widehat{T}_{n,n}[f]$, $n = 2^k$, $k = 1, 2, \dots, 9$, for $m = j/2$, $j = 3, 4, \dots, 12$. Table 2 presents the numbers

$$\mu_{m,k} = \frac{1}{\log 2} \cdot \log \left(\frac{|\widehat{T}_{2^k}[f] - I[f]|}{|\widehat{T}_{2^{k+1}}[f] - I[f]|} \right),$$

for the same values of m and for $k = 1, 2, \dots, 8$. It is seen that, with increasing k , the $\mu_{m,k}$ are tending to $4m + 4$ when $2m$ is an odd integer and to $2m + 2$ otherwise, completely in accordance with Theorem 3.3. (With the floating-point arithmetic we are using, this convergence seems to be less visible for relatively large m for which $2m$ is an odd integer, however.)

4. Further improvement for smooth $f(Q)$

In the preceding section, we showed that, in case of smooth $f(Q)$, the performance of $\widehat{T}_{n,n'}[f]$ can be improved substantially by choosing $\psi(t) \in \mathcal{S}_m$ with $2m$

Table 1

Relative errors in the rules $\widehat{T}_n[f] = \widehat{T}_{n,n}[f]$ for the integral of Section 3.1, obtained with $n = 2^k$, $k = 1(1)10$, and with the \sin^m -transformation using $m = 1.5(0.5)6$

n	$m = 1.5$	$m = 2.0$	$m = 2.5$	$m = 3.0$	$m = 3.5$	$m = 4.0$	$m = 4.5$	$m = 5.0$	$m = 5.5$	$m = 6.0$
2	4.40D–01	3.77D–01	3.20D–01	2.66D–01	2.17D–01	1.70D–01	1.25D–01	8.29D–02	4.24D–02	3.54D–03
4	1.20D–01	1.82D–01	2.28D–01	2.57D–01	2.72D–01	2.76D–01	2.71D–01	2.60D–01	2.44D–01	2.26D–01
8	2.27D–06	2.26D–04	1.44D–03	4.29D–03	9.05D–03	1.57D–02	2.42D–02	3.42D–02	4.54D–02	5.75D–02
16	7.33D–07	1.24D–06	6.71D–07	1.30D–07	1.85D–06	6.95D–06	1.68D–05	3.22D–05	5.23D–05	7.43D–05
32	2.67D–11	7.85D–09	2.70D–11	5.62D–11	2.67D–11	2.72D–11	2.26D–11	1.56D–11	3.60D–12	1.08D–11
64	3.82D–16	1.22D–10	1.33D–19	3.22D–13	1.53D–19	1.45D–15	1.52D–19	9.80D–18	9.74D–20	1.90D–20
128	3.72D–19	1.90D–12	1.19D–24	1.25D–15	1.31D–29	1.41D–18	3.36D–34	2.40D–21	0.00D+00	5.80D–24
256	3.63D–22	2.97D–14	7.22D–29	4.89D–18	3.36D–34	1.37D–21	5.04D–34	5.85D–25	0.00D+00	3.52D–28
512	3.55D–25	4.64D–16	3.70D–33	1.91D–20	6.72D–34	1.34D–24	6.72D–34	1.43D–28	1.68D–34	2.10D–32

Table 2

The numbers $\mu_{m,k} = \frac{1}{\log 2} \cdot \log \left(\frac{|\widehat{T}_{2^k}[f]/I[f]|}{|\widehat{T}_{2^{k+1}}[f]-I[f]|} \right)$, for $k = 1(1)9$ and $m = 1.5(0.5)6$, for the integral of Section 3.1, where $\widehat{T}_n[f]$ are those of Table 1

k	m = 1.5	m = 2.0	m = 2.5	m = 3.0	m = 3.5	m = 4.0	m = 4.5	m = 5.0	m = 5.5	m = 6.0
1	1.871	1.053	0.488	0.049	-0.331	-0.702	-1.114	-1.648	-2.527	-5.996
2	15.698	9.649	7.310	5.907	4.911	4.131	3.485	2.925	2.427	1.973
3	1.628	7.510	11.065	15.010	12.255	11.144	10.493	10.054	9.762	9.596
4	14.747	7.306	14.598	11.174	16.080	17.963	19.503	20.980	23.791	22.711
5	16.089	6.011	27.594	7.450	27.379	14.196	27.149	20.597	25.141	29.083
6	10.004	6.001	16.780	8.004	33.442	10.008	49.684	11.994	49.042	11.680
7	10.001	6.000	14.004	8.001	16.253	10.002	*	12.004	*	14.006
8	10.001	6.001	14.184	8.001	*	10.001	*	11.996	*	14.046

an odd integer. In this section, we continue our treatment of smooth integrands by improving further the performance of the rule $\widehat{T}_{n,n'}$. As mentioned in the remark in Appendix C, it is desirable to get as much accuracy out of $\widehat{T}_{n,n'}$ for a given amount of clustering of the transformed abscissas on U . As in the preceding section, this can be achieved for special values of m , provided the integrand is preprocessed suitably.

Let

$$p(z) = Az + B;$$

$$A = \frac{w(0, 0, 1) - w(0, 0, -1)}{2}, \quad B = \frac{w(0, 0, 1) + w(0, 0, -1)}{2}.$$

Then $p(\pm 1) = w(0, 0, \pm 1)$. By the fact that $I[f] = \int_0^\pi \left[\int_0^{2\pi} w(x, y, z) d\phi \right] \sin \theta d\theta$, we can also write

$$I[f] = J[w - p] + J[p];$$

$$J[w - p] = \int_0^\pi \left[\int_0^{2\pi} \{w(x, y, z) - p(z)\} d\phi \right] \sin \theta d\theta,$$

$$J[p] = \int_0^\pi \left[\int_0^{2\pi} p(z) d\phi \right] \sin \theta d\theta = 4\pi B = 2\pi[w(0, 0, 1) + w(0, 0, -1)].$$

We now apply the product trapezoidal rule to the integral $J[w - p]$, to obtain $\widehat{T}_{n,n'}[f - p/R]$ as the approximation to $J[w - p] = I[f - p/R]$. Thus, the approximation to $I[f]$ is the rule

$$\check{T}_{n,n'}[f] = \widehat{T}_{n,n'}[f - p/R] + J[p]$$

that is also given as in

$$\check{T}_{n,n'}[f] = \widehat{T}_{n,n'}[f] + 4\pi B - 2\pi B \left[h \sum_{j=1}^{n-1} \sin(\Psi(j/n)) \Psi'(j/n) \right]. \tag{4.1}$$

This follows from the fact that, for the function $u(x, y, z) = z$, $\widehat{T}_{n,n'}[u/R] = 0$. Here, we recall that $\Psi(t) = \pi\psi(t)$ with $\psi \in \mathcal{S}_m$.

The analysis of this rule is identical to that of $\widehat{T}_{n,n'}[f]$; we just have to replace $w(x, y, z)$ by $w(x, y, z) - p(z)$ everywhere. Because

$$p(z) = w(0, 0, 1) + A(z - 1) = w(0, 0, -1) + A(z + 1),$$

we have, in the notation of Section 3,

$$w(x, y, z) - p(z) \sim -A(z - 1) + \sum_{\substack{i, j, k \geq 0 \\ i+j+k \geq 1}} \frac{w^{(i, j, k)}(0, 0, 1)}{i!j!k!} x^i y^j (z - 1)^k \quad \text{as } \theta \rightarrow 0,$$

$$w(x, y, z) - p(z) \sim -A(z + 1) + \sum_{\substack{i, j, k \geq 0 \\ i+j+k \geq 1}} \frac{w^{(i, j, k)}(0, 0, -1)}{i!j!k!} x^i y^j (z + 1)^k \quad \text{as } \theta \rightarrow \pi.$$

Note that, in these asymptotic expansions, the terms $w^{(0,0,0)}(0, 0, \pm 1)$ have disappeared and the terms $w^{(0,0,1)}(0, 0, \pm 1)(z \mp 1)$ have been modified to read $[w^{(0,0,1)}(0, 0, \pm 1) - A](z \mp 1)$.

Let now $F^{\text{imp}}(\theta, \phi) = F(\theta, \phi) - p(z)\sin\theta$ and $v^{\text{imp}}(\theta) = \int_0^{2\pi} F^{\text{imp}}(\theta, \phi) d\phi$, so that $J[w - p] = \int_0^\pi v^{\text{imp}}(\theta) d\theta$. With this notation, Theorem 3.2 is modified as follows:

Theorem 4.1. *When $f(\xi, \eta, \zeta)$ is smooth over S , $v^{\text{imp}}(\theta)$ has the asymptotic expansions*

$$\begin{aligned} v^{\text{imp}}(\theta) &\sim \sum_{\substack{i, j, k \geq 0 \\ i+j+k \geq 1}} \tilde{A}_{i, j, k}^{(+)}(\sin \theta)^{2i+2j+1} (\cos \theta - 1)^k \quad \text{as } \theta \rightarrow 0, \\ v^{\text{imp}}(\theta) &\sim \sum_{\substack{i, j, k \geq 0 \\ i+j+k \geq 1}} \tilde{A}_{i, j, k}^{(-)}(\sin \theta)^{2i+2j+1} (\cos \theta + 1)^k \quad \text{as } \theta \rightarrow \pi, \end{aligned} \tag{4.2}$$

where

$$\tilde{A}_{0,0,1}^{(\pm)} = A_{0,0,1}^{(\pm)} - 2\pi A; \quad \tilde{A}_{i, j, k}^{(\pm)} = A_{i, j, k}^{(\pm)} \quad \text{when } (i, j, k) \neq (0, 0, 1),$$

with $A_{i, j, k}^{(\pm)}$ as in Theorem 3.2. Consequently,

$$\begin{aligned} v^{\text{imp}}(\theta) &\sim \sum_{i=1}^{\infty} \mu_i^{(+)} \theta^{2i+1} \quad \text{as } \theta \rightarrow 0; \\ v^{\text{imp}}(\theta) &\sim \sum_{i=1}^{\infty} \mu_i^{(-)} (\pi - \theta)^{2i+1} \quad \text{as } \theta \rightarrow \pi, \end{aligned} \tag{4.3}$$

for some constants $\mu_i^{(\pm)}$.

As can be seen from (4.3), the asymptotic expansions of $v^{\text{imp}}(\theta)$ as $\theta \rightarrow 0$ and $\theta \rightarrow \pi$ start with the terms θ^3 and $(\pi - \theta)^3$, respectively, the next terms being θ^5 and $(\pi - \theta)^5$. In view of this, and by Theorem C.1, we have the following optimal result concerning the rule $\check{T}_{n,n'}[f]$ that approximates $I[f]$:

Theorem 4.2. *With $\psi(t)$, in \mathcal{S}_m , and with $n' \sim \alpha n^\beta$ as $n \rightarrow \infty$ for some fixed positive α and β , there holds*

$$\check{T}_{n,n'}[f] - I[f] = \begin{cases} O(h^{6m+6}) & \text{as } h \rightarrow 0, \text{ if } 4m \text{ odd integer,} \\ O(h^{4m+4}) & \text{as } h \rightarrow 0, \text{ otherwise.} \end{cases}$$

When $4m$ is an odd integer, we also have the complete asymptotic expansion

$$\begin{aligned} \check{T}_{n,n'}[f] \sim I[f] &+ \sum_{i=0}^{\infty} \sigma_i h^{6m+6+2i} + \sum_{i=0}^{\infty} \sigma'_i h^{8m+8+2i} \\ &+ \sum_{i=0}^{\infty} \sigma''_i h^{10m+10+2i} \quad \text{as } h \rightarrow 0. \end{aligned}$$

For example, in case $m = 0.25$, the expansion in this theorem contains the powers $h^{7.5}, h^{9.5}, h^{10}, h^{11.5}, h^{12}, h^{12.5}, \dots$

4.1. A numerical example

We have applied the improved method above to the example of Section 3.1. The transformation we use for the variable θ is again the \sin^m -transformation for various values of m .

The numerical results in Tables 3 and 4, which were computed in quadruple-precision arithmetic, illustrate the result of Theorem 4.2 very clearly. Table 3 gives the relative errors in the $\check{T}_n[f] \equiv \check{T}_{n,n}[f]$, $n = 2^k$, $k = 1, 2, \dots, 9$, for $m = -0.25$ and $m = 0.25(0.25)2.25$. Table 4 presents the numbers

$$\mu_{m,k} = \frac{1}{\log 2} \cdot \log \left(\frac{|\check{T}_{2^k}[f] - I[f]|}{|\check{T}_{2^{k+1}}[f] - I[f]|} \right),$$

for the same values of m and for $k = 1, 2, \dots, 8$. It is seen that, with increasing k , the $\mu_{m,k}$ are tending to $6m + 6$ when $4m$ an odd integer, that is, when $m = j/2 - 3/4$, $j = 1, 2, \dots$, and to $4m + 4$ otherwise, completely in accordance with Theorem 4.2. (With the floating-point arithmetic we are using, this convergence seems to be less visible for relatively large m for which $4m$ is an odd integer, however.)

We would like to note also that, when $m = -0.25$, class \mathcal{S}_m variable transformations have asymptotic behavior $\psi(t) \sim \alpha t^{0.75}$ as $t \rightarrow 0+$ and $\psi(t) \sim 1 - \alpha(1 - t)^{0.75}$ as $t \rightarrow 1-$. This means that the transformed abscissas $\theta_j = \Psi(j/n)$

Table 3

Relative errors in the rules $\tilde{T}_n[f] = \tilde{T}_{n,n}[f]$ for the integral of Sections 3.1 and 4.1, obtained with $n = 2^k$, $k = 1(1)9$, and with the \sin^m -transformation using $m = -0.25$ and $m = 0.25(0.25)2.25$

n	$m = -0.25$	$m = 0.25$	$m = 0.5$	$m = 0.75$	$m = 1$	$m = 1.25$	$m = 1.5$	$m = 1.75$	$m = 2.0$	$m = 2.25$
2	2.84D+00	9.10D+00	1.17D+01	1.42D+01	1.64D+01	1.85D+01	2.05D+01	2.23D+01	2.41D+01	2.58D+01
4	3.73D-01	2.98D-01	4.07D-01	7.01D-01	1.14D+00	1.67D+00	2.27D+00	2.89D+00	3.53D+00	4.17D+00
8	4.69D-03	4.19D-03	4.01D-03	3.95D-03	3.09D-03	1.50D-03	4.46D-05	1.58D-04	3.51D-03	1.18D-02
16	2.97D-05	1.35D-05	1.11D-05	1.35D-05	1.35D-05	1.34D-05	1.34D-05	1.35D-05	1.35D-05	1.32D-05
32	6.20D-07	7.20D-10	3.68D-08	4.96D-10	8.26D-10	4.96D-10	4.91D-10	4.96D-10	4.96D-10	4.96D-10
64	2.59D-08	1.22D-12	5.82D-10	2.36D-16	1.28D-12	2.68D-18	4.94D-15	2.81D-18	3.24D-17	2.81D-18
128	1.12D-09	6.70D-15	9.09D-12	1.65D-19	5.00D-15	1.07D-23	4.81D-18	1.45D-27	7.16D-21	3.57D-31
256	4.93D-11	3.70D-17	1.42D-13	1.14D-22	1.95D-17	9.20D-28	4.69D-21	4.31D-32	1.75D-24	0.00D+00
512	2.17D-12	2.04D-19	2.22D-15	7.85D-26	7.63D-20	4.31D-32	4.58D-24	2.47D-32	4.26D-28	3.08D-33

Table 4

The numbers $\mu_{m,k} = \frac{1}{\log 2} \cdot \log \left(\frac{|\tilde{T}_{2^k}[f]-I[f]|}{|\tilde{T}_{2^{k+1}}[f]-I[f]|} \right)$, for $k = 1(1)9$ and $m = -0.25$ and $m = 0.25(0.25)2.25$, for the integral of Sections 3.1 and 4.1, where $\tilde{T}_n[f]$ are those of Table 3

k	$m = -0.25$	$m = 0.25$	$m = 0.5$	$m = 0.75$	$m = 1$	$m = 1.25$	$m = 1.5$	$m = 1.75$	$m = 2.0$	$m = 2.25$
1	2.925	4.932	4.850	4.338	3.851	3.468	3.176	2.950	2.772	2.629
2	6.313	6.152	6.667	7.471	8.523	10.123	15.634	14.159	9.973	8.470
3	7.305	8.279	8.503	8.198	7.836	6.801	1.729	3.554	8.029	9.795
4	5.581	14.193	8.230	14.728	14.000	14.727	14.741	14.728	14.727	14.705
5	4.581	9.209	5.983	21.001	9.332	27.461	16.602	27.396	23.870	27.396
6	4.529	7.505	6.001	10.485	8.002	17.940	10.004	30.850	12.141	42.837
7	4.510	7.501	6.000	10.501	8.000	13.503	10.001	15.038	12.002	*
8	4.504	7.500	6.000	10.500	8.000	14.280	10.000	0.893	12.001	*

are not clustered near the endpoints $\theta = 0$ and $\theta = \pi$; in fact, the θ_j are less dense at the endpoints than in the middle of $[0, \pi]$ in this case.

5. Concluding remarks

In this work, we have described numerical quadrature formulas based on the trapezoidal rule for computing integrals of smooth functions over smooth surfaces in \mathbb{R}^3 that are homeomorphic to the unit sphere. These formulas are obtained as follows: We first transform the integrals to the unit sphere, and express them in terms of the standard spherical coordinates θ and ϕ , $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$. We then transform the variable θ via $\theta = \pi\psi(t)$, $0 \leq t \leq 1$, where $\psi(t)$ is a transformation in the class \mathcal{S}_m . Finally, we apply the product trapezoidal rule to the integral in t and ϕ . We have shown that, when $2m$ is an odd integer, the error in this formula is $O(h^{4m+4})$. We have also described an improved method, based on the same quadrature formula, in which we first subtract from the integrand a suitable function (depending on the integrand and the surface on which we are integrating), whose integral is known, and apply the same product trapezoidal rule above to this preprocessed integrand. This time, the error is $O(h^{6m+6})$, provided m is chosen such that $4m$ is an odd integer.

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Appendix A. Euler–Maclaurin expansions

Euler–Maclaurin expansions concerning the trapezoidal rule approximations of finite-range integrals $\int_a^b u(x) dx$ are the main analytical tool we use in our study. For the sake of easy reference, we reproduce here the relevant Euler–Maclaurin expansions as Theorems A.1 and A.2. Of these, Theorem A.1, concerns the integrals $\int_a^b u(x) dx$ in the case the integrands $u(x)$ are in $C^{2m}[a, b]$; this theorem can be found in most books on numerical analysis. See, for example, Davis and Rabinowitz [5], Ralston and Rabinowitz [13], and Atkinson [1]. See also the brief review in Sidi [20, Appendix D]. Theorem A.2 is a special case of a very general theorem from Sidi [21], and is expressed in terms of the asymptotic expansions of $u(x)$ as $x \rightarrow a+$ and $x \rightarrow b-$ and is easy to write down and use.

Theorem A.1. Let $u \in C^{2m}[a, b]$, and let $h = (b - a)/n$ for $n = 1, 2, \dots$. Then

$$h \sum_{i=0}^{n-1} u(a + ih) = \int_a^b u(x) dx + \sum_{k=1}^{m-1} \frac{B_{2k}}{(2k)!} [u^{(2k-1)}(b) - u^{(2k-1)}(a)] h^{2k} + (b - a) \frac{B_{2m}}{(2m)!} u^{(2m)}(\xi_{m,n}) h^{2m} \quad \text{for some } \xi_{m,n} \in (a, b).$$

Here, B_s is the s th Bernoulli number.

Theorem A.2. Let $u \in C^\infty(a, b)$, and assume that $u(x)$ has the asymptotic expansions

$$u(x) \sim \sum_{s=0}^{\infty} c_s (x - a)^{\gamma_s} \quad \text{as } x \rightarrow a+,$$

$$u(x) \sim \sum_{s=0}^{\infty} d_s (b - x)^{\delta_s} \quad \text{as } x \rightarrow b-,$$

where the γ_s and δ_s are distinct complex numbers that satisfy

$$-1 < \Re\gamma_0 \leq \Re\gamma_1 \leq \Re\gamma_2 \leq \dots; \quad \lim_{s \rightarrow \infty} \Re\gamma_s = +\infty,$$

$$-1 < \Re\delta_0 \leq \Re\delta_1 \leq \Re\delta_2 \leq \dots; \quad \lim_{s \rightarrow \infty} \Re\delta_s = +\infty.$$

Assume furthermore that, for each positive integer k , $u^{(k)}(x)$ has asymptotic expansions as $x \rightarrow a+$ and $x \rightarrow b-$ that are obtained by differentiating those of $u(x)$ term by term k times. Let also $h = (b - a)/n$ for $n = 1, 2, \dots$. Then

$$h \sum_{i=1}^{n-1} u(a + ih) \sim \int_a^b u(x) dx + \sum_{\substack{s=0 \\ \gamma_s \notin \{2,4,6,\dots\}}}^{\infty} c_s \zeta(-\gamma_s) h^{\gamma_s+1} + \sum_{\substack{s=0 \\ \delta_s \notin \{2,4,6,\dots\}}}^{\infty} d_s \zeta(-\delta_s) h^{\delta_s+1} \quad \text{as } h \rightarrow 0,$$

where $\zeta(z)$ is the Riemann Zeta function.

It is clear from Theorem A.2 that the even powers of $(x - a)$ and $(b - x)$, if present in the asymptotic expansions of $u(x)$ as $x \rightarrow a+$ and $x \rightarrow b-$, do not contribute to the asymptotic expansion of $h \sum_{i=1}^{n-1} u(a + ih)$ as $h \rightarrow 0$.

In addition, if γ_p is the first of the γ_s that is different from $2, 4, 6, \dots$, and if δ_q is the first of the δ_s that is different from $2, 4, 6, \dots$, then we have the useful observation that

$$h \sum_{i=1}^{n-1} u(a + ih) - \int_a^b u(x) dx = O(h^{\sigma+1}) \quad \text{as } h \rightarrow 0; \quad \sigma = \min\{\Re\gamma_p, \Re\delta_q\}.$$

Appendix B. Extended class \mathcal{S}_m transformations

Definition B.1. A function $\psi(t)$ is in the extended class \mathcal{S}_m , m arbitrary, if it has the following properties:

1. $\psi \in C[0, 1]$ and $\psi \in C^\infty(0, 1)$; $\psi(0) = 0$, $\psi(1) = 1$, and $\psi'(t) > 0$ on $(0, 1)$.
2. $\psi'(t)$ is symmetric with respect to $t = 1/2$; that is, $\psi'(1 - t) = \psi'(t)$. Consequently, $\psi(1 - t) = 1 - \psi(t)$.
3. $\psi'(t)$ has the following asymptotic expansions as $t \rightarrow 0+$ and $t \rightarrow 1-$:

$$\psi'(t) \sim \sum_{i=0}^{\infty} \epsilon_i t^{m+2i} \quad \text{as } t \rightarrow 0+; \tag{B.1}$$

$$\psi'(t) \sim \sum_{i=0}^{\infty} \epsilon_i (1 - t)^{m+2i} \quad \text{as } t \rightarrow 1-,$$

the ϵ_i being the same in both expansions, and $\epsilon_0 > 0$. Consequently,

$$\psi(t) \sim \sum_{i=0}^{\infty} \epsilon_i \frac{t^{m+2i+1}}{m + 2i + 1} \quad \text{as } t \rightarrow 0+, \tag{B.2}$$

$$\psi(t) \sim 1 - \sum_{i=0}^{\infty} \epsilon_i \frac{(1 - t)^{m+2i+1}}{m + 2i + 1} \quad \text{as } t \rightarrow 1-.$$

4. Furthermore, for each positive integer k , $\psi^{(k)}(t)$ has asymptotic expansions as $t \rightarrow 0+$ and $t \rightarrow 1-$ that are obtained by differentiating those of $\psi(t)$ term by term k times.

The difference between Definition B.1 and the definition of the class \mathcal{S}_m in [17] is that m is a positive integer in the latter, hence $\psi \in C^\infty[0, 1]$. In Definition B.1, $\psi(t)$ is not infinitely differentiable at $t = 0$ and $t = 1$ when m is not a positive integer. The fact that we are now allowing m to assume arbitrary values has a beneficial effect, as we will see in Appendix C.

As was mentioned in [17], the fact that $\psi'(t)$ has the asymptotic expansions given in (B.1)—with consecutive powers of t and $(1 - t)$ there increasing by 2 instead of by 1—is the most important aspect of the extended class \mathcal{S}_m .

The following result shows that the family of the extended classes \mathcal{S}_m is closed with respect to composition.

Lemma B.2. Let $\psi_i \in \mathcal{S}_{m_i}$, $i = 1, \dots, r$, and define $\Psi(t) = \psi_1(\psi_2(\dots(\psi_r(t))\dots))$. Then $\Psi \in \mathcal{S}_M$ with $M = \prod_{i=1}^r (m_i + 1) - 1$.

Before proceeding further, we mention that in case the integrand $f(x)$ in the integral $\int_0^1 f(x) dx$ is smooth in $[0, 1]$, and we let $x = \psi(t)$ with $\psi \in \mathcal{S}_m$, then excellent approximations are obtained by applying the trapezoidal rule to the

transformed integral $\int_0^1 f(\psi(t))\psi'(t) dt$ when m is even, and the error in this approximation is at worst $O(n^{-2m-2})$ as $n \rightarrow \infty$, where $n + 1$ is the number of abscissas in the approximation, as shown in [17]. Now, by (B.2), $\psi \in \mathcal{S}_m$ behaves asymptotically (in a polynomial fashion) as in

$$\psi(t) \sim \alpha t^{m+1} \text{ as } t \rightarrow 0, \quad \psi(t) \sim 1 - \alpha(1 - t)^{m+1} \text{ as } t \rightarrow 1.$$

If, instead of class \mathcal{S}_m transformations, we use the Korobov transformation that also behaves asymptotically in the same way, the error in the resulting approximations to $\int_0^1 f(x) dx$ is at worst $O(n^{-m-2})$ as $n \rightarrow \infty$, when m is even. This shows that class \mathcal{S}_m transformations have more useful approximation properties.

B.1. The extended \sin^m -transformation

The extended \sin^m -transformation, just as the original \sin^m -transformation, is defined via

$$\psi_m(t) = \frac{\Theta_m(t)}{\Theta_m(1)}; \quad \Theta_m(t) = \int_0^t (\sin \pi u)^m du. \tag{B.3}$$

From the equality

$$\Theta_m(t) = \frac{m-1}{m} \Theta_{m-2}(t) - \frac{1}{\pi m} (\sin \pi t)^{m-1} \cos \pi t,$$

which can be obtained by integration by parts, we have the recursion relation

$$\psi_m(t) = \psi_{m-2}(t) - \frac{\Gamma(\frac{m}{2})}{2\sqrt{\pi}\Gamma(\frac{m+1}{2})} (\sin \pi t)^{m-1} \cos \pi t. \tag{B.4}$$

Note that $\psi_m(t)$ is related to $\psi_{m-2}(t)$ but not to $\psi_{m-1}(t)$.

When m is a positive integer, (B.4) can be used to compute $\psi_m(t)$ with the initial conditions

$$\psi_0(t) = t \text{ and } \psi_1(t) = \frac{1}{2}(1 - \cos \pi t). \tag{B.5}$$

Thus, in this case, $\psi_m(t)$ can be expressed in terms of elementary functions.

For noninteger m , however, $\psi_m(t)$ cannot be expressed in terms of elementary functions. Even so, it can be computed rather easily in different ways. One of the ways is by computing the integral representation of $\Theta_m(t)$ by Gauss–Jacobi quadrature when m is real. This, of course, requires the availability of the abscissas and weights of the appropriate quadrature rules.

Another way that requires no tables makes use of the fact that $\Theta_m(t)$ can be represented in terms of the Gauss hypergeometric function $F(a, b; c; z)$, which is defined via the power series

$$F(a, b; c; z) = \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(c)_k} \frac{z^k}{k!},$$

where $(x)_0 = 1$ and $(x)_k = x(x + 1) \cdots (x + k - 1)$ for $k = 1, 2, \dots$. The fact that the k th term of this series tends to zero practically like z^k when $|z| < 1$, suggests that some of the power series representations of $\Theta_m(t)$ can also be used to compute $\Theta_m(t)$ for noninteger m . The details follow.

By the fact that $\Theta'_m(t) = (\sin \pi t)^m$ is symmetric with respect to $t = 1/2$, we have that $\Theta_m(t) = \Theta_m(1) - \Theta_m(1 - t)$ for $t \in [1/2, 1]$ and thus $\Theta_m(1) = 2\Theta_m(1/2)$ as well. Thus, it is enough to know $\Theta_m(t)$ for $t \in [0, 1/2]$. Consequently,

$$\psi_m(t) = \frac{\Theta_m(t)}{2\Theta_m(1/2)} \text{ for } t \in [0, 1/2]; \quad \psi_m(t) = 1 - \psi_m(1 - t) \text{ for } t \in [1/2, 1].$$

Therefore, it is enough to consider the computation of $\Theta_m(t)$ only for $t \in [0, 1/2]$.

We first have

$$\Theta_m(t) = \frac{(2S)^{m+1}}{\pi(m+1)} F\left(\frac{1}{2} - \frac{1}{2}m, \frac{1}{2}m + \frac{1}{2}; \frac{1}{2}m + \frac{3}{2}; S^2\right); \quad S = \sin \frac{\pi t}{2}. \quad (\text{B.6})$$

Now, the terms in the expansion of $F(\frac{1}{2} - \frac{1}{2}m, \frac{1}{2}m + \frac{1}{2}; \frac{1}{2}m + \frac{3}{2}; S^2)$ in powers of S^2 are all of the same sign for $k \geq \lfloor (m + 1)/2 \rfloor$. In addition, the k th term is $O(k^{-(m+3)/2} S^{2k})$ as $k \rightarrow \infty$ and, by the fact that $0 \leq S \leq \sin(\pi/4) = 1/\sqrt{2}$ when $t \in [0, 1/2]$, it is $O(k^{-(m+3)/2} 2^{-k})$ at worst. This gives us a quickly converging expansion for $\Theta_m(t)$ that can be used for the actual computation of $\Theta_m(t)$. Furthermore, we can also use a nonlinear sequence transformation, such as that of Shanks [16] (or the equivalent ϵ -algorithm of Wynn [25]) or of Levin [11], to accelerate the convergence of this expansion. Both transformations are treated in detail in the recent book by Sidi [20].

Next, we have

$$\Theta_m(t) = \frac{2T}{\pi(m+1)} \left(\frac{2T}{1+T^2}\right)^m F\left(1, \frac{1}{2} - \frac{1}{2}m; \frac{1}{2}m + \frac{3}{2}; -T^2\right); \quad T = \tan \frac{\pi t}{2}. \quad (\text{B.7})$$

The k th term, in the expansion of $F(1, \frac{1}{2} - \frac{1}{2}m; \frac{1}{2}m + \frac{3}{2}; -T^2)$ in powers of T^2 is $O(k^{-m-1} T^{2k})$ as $k \rightarrow \infty$. Consequently, this expansion converges slowly for t close to $1/2$ because $T \rightarrow 1$ as $t \rightarrow 1/2$. However, it is an essentially alternating series since its terms, for $k \geq \lfloor (m + 1)/2 \rfloor$, alternate in sign. Consequently, we can apply to it the Shanks or the Levin transformation and obtain its sum to machine precision using a very small number of its terms, and in an absolutely stable fashion. Indeed, using the Levin transformation, $\Theta_m(t)$ can be computed with an accuracy of almost thirty five digits by using only the first twenty five terms of the expansion of $F(1, \frac{1}{2} - \frac{1}{2}m; \frac{1}{2}m + \frac{3}{2}; -T^2)$.

Appendix C. Convergence of the trapezoidal rule with extended class \mathcal{S}_m transformations

In this appendix, we summarize the results of [22] concerning the convergence of the trapezoidal rule in conjunction with variable transformations in the extended class \mathcal{S}_m . In the sequel, we will call the *extended class* \mathcal{S}_m simply the *class* \mathcal{S}_m .

Theorem C.1. *Let the function $f(x)$ be in $C^\infty(0, 1)$, and assume that $f(x)$ has the asymptotic expansions*

$$f(x) \sim \sum_{s=0}^{\infty} c_s x^{\gamma_s} \text{ as } x \rightarrow 0+; \quad f(x) \sim \sum_{s=0}^{\infty} d_s (1-x)^{\delta_s} \text{ as } x \rightarrow 1-.$$

Here γ_s and δ_s are distinct complex numbers that satisfy

$$\begin{aligned} -1 < \Re\gamma_0 \leq \Re\gamma_1 \leq \Re\gamma_2 \leq \dots; \quad \lim_{s \rightarrow \infty} \Re\gamma_s = +\infty, \\ -1 < \Re\delta_0 \leq \Re\delta_1 \leq \Re\delta_2 \leq \dots; \quad \lim_{s \rightarrow \infty} \Re\delta_s = +\infty. \end{aligned}$$

Assume furthermore that, for each positive integer k , $f^{(k)}(x)$ has asymptotic expansions as $x \rightarrow 0+$ and $x \rightarrow 1-$ that are obtained by differentiating those of $f(x)$ term by term k times. Let $I[f] = \int_0^1 f(x) dx$, and let us now make the transformation of variable $x = \psi(t)$, where $\psi \in \mathcal{S}_m$, in $I[f]$. Finally, let us approximate $I[f]$ via the trapezoidal rule $\widehat{Q}_n[f] = \sum_{i=1}^{n-1} f(\psi(ih))\psi'(ih)$, where $h = 1/n$, $n = 1, 2, \dots$. Then the following hold:

(i) *In the worst case,*

$$\widehat{Q}_n[f] - I[f] = O(h^{(\omega+1)(m+1)}) \text{ as } h \rightarrow 0; \quad \omega = \min\{\Re\gamma_0, \Re\delta_0\}.$$

(ii) *Let us merge the sets $C = \{\gamma_0, \gamma_1, \dots\}$ and $D = \{\delta_0, \delta_1, \dots\}$ to obtain the set $B = \{\beta_0, \beta_1, \dots\}$, such that (i) β_s are distinct, (ii) $\Re\beta_0 \leq \Re\beta_1 \leq \dots$, and (iii) $\alpha \in B$ if and only if $\alpha \in C$ or $\alpha \in D$. Then, if β_0 is real, and if $m = (q - \beta_0)/(1 + \beta_0)$, where q is an arbitrary even integer, then the preceding result is improved to read at worst*

$$\widehat{Q}_n[f] - I[f] = O(h^{(\beta_1+1)(m+1)}) \text{ as } h \rightarrow 0.$$

Thus, in case γ_0 and δ_0 are real and $\gamma_0 = \delta_0$, hence $\beta_0 = \gamma_0 = \delta_0$, there holds

$$\widehat{Q}_n[f] - I[f] = O(h^{(\omega+1)(m+1)}) \text{ as } h \rightarrow 0; \quad \omega = \min\{\Re\gamma_1, \Re\delta_1\}.$$

Remark. The fact that $\psi(t) \sim \alpha t^{m+1}$ as $t \rightarrow 0+$ implies that, when m is large, the abscissas of the rule $\widehat{Q}_n[f]$, namely, $x_i \equiv \psi(ih) = \psi(i/n)$ in the original variable of integration x , are clustered in two very small regions, one to the right of $x = 0$ and the other to the left of $x = 1$, many of them being very close to 0

and to 1. The amount of this clustering is determined by the size of m ; the larger m , the larger the density of the x_i near $x = 0$ and $x = 1$. As the clustering gets larger, the numerical computation of the rule $\widehat{Q}_n[f]$ in finite-precision arithmetic may become problematic due to possible underflows and overflows in case $f(x)$ has endpoint singularities. From this, we conclude that too much clustering is not desirable. Thus, for a given m (that is, for a given amount of clustering), we would like to get as high an accuracy as possible out of $\widehat{Q}_n[f]$.

The situations described in the corollary below arise, for example, in case $f(x)$ is infinitely differentiable on $[0, 1]$. The quality of $\widehat{Q}_n[f]$ in this corollary is best possible, by the preceding remark.

Corollary C.2. *Assume $f(x)$ is as in Theorem C.1, and let the β_i be as in part (ii) there.*

- (i) *In case $\beta_0 = 0$ and $\beta_1 = 1$, if we choose m to be an even integer, we have $\widehat{Q}_n[f] - I[f] = O(h^{2m+2})$ as $h \rightarrow 0$.*
- (ii) *In case $\beta_0 = 1$ and $\beta_1 = 2$, if we choose $2m$ to be an odd integer, we have $\widehat{Q}_n[f] - I[f] = O(h^{3m+3})$ as $h \rightarrow 0$.*
- (iii) *In case $\beta_0 = 1$ and $\beta_1 = 3$, if we choose $2m$ to be an odd integer, we have $\widehat{Q}_n[f] - I[f] = O(h^{4m+4})$ as $h \rightarrow 0$.*

Note that part (i) of the corollary applies when $|f(0)| + |f(1)| \neq 0$ and $|f'(0)| + |f'(1)| \neq 0$. Part (ii) applies when $f(0) = f(1) = 0$, $|f'(0)| + |f'(1)| \neq 0$, and $|f''(0)| + |f''(1)| \neq 0$. Part (iii) applies when $f(0) = f(1) = 0$, $|f'(0)| + |f'(1)| \neq 0$, $f''(0) = f''(1) = 0$, and $|f'''(0)| + |f'''(1)| \neq 0$.

Thus, the result of part (i) of Corollary C.2, despite being quite good, is nevertheless inferior to those of parts (ii) and (iii). That is, the best accuracy that can be achieved by $\widehat{Q}_n[f]$ when $|f(0)| + |f(1)| \neq 0$ and $|f'(0)| + |f'(1)| \neq 0$ is less than those achieved when $f(0) = f(1) = 0$. The next theorem shows how this situation can be improved in a simple way.

Theorem C.3. *Assume $f(x)$ is in $C^\infty[0, 1]$, and that $|f(0)| + |f(1)| \neq 0$, that is, at least one of $f(0)$ and $f(1)$ is nonzero. Let $p(x)$ be the linear function that interpolates $f(x)$ at $x = 0$ and $x = 1$, and let $u(x) = f(x) - p(x)$. Next, transform the variable x in the integral $\int_0^1 u(x) dx$ via $x = \psi(t)$, where $\psi \in \mathcal{S}_m$, and approximate the transformed integral by the trapezoidal rule. Denote the resulting approximations by $\widehat{Q}_n[u]$. Then*

$$\left\{ \widehat{Q}_n[u] + \frac{1}{2}[f(0) + f(1)] \right\} - I[f] = \begin{cases} O(h^{3m+3}) & \text{as } h \rightarrow 0, \text{ if } 2m \text{ odd integer,} \\ O(h^{2m+2}) & \text{as } h \rightarrow 0, \text{ otherwise.} \end{cases}$$

In case only one of $f(0)$ and $f(1)$ vanishes, and a few other special conditions hold, we can use another approach, quite different from that described in Theorem C.3. We give this approach next. Note the unusual application of the class \mathcal{S}_m transformations.

Theorem C.4. *Assume $f \in C^\infty[0, 1]$, and that only one of $f(0)$ and $f(1)$ vanishes. Let $f(0) = 0$, without loss of generality, and assume that $f^{(i)}(0) = 0$ for $2 \leq i \leq j-1$, and $f^{(j)}(0) \neq 0$ for some $j \geq 2$. Assume also that $f^{(2k+1)}(1) = 0$, $k = 0, 1, \dots$. Let $\psi(t)$ be in \mathcal{S}_m for some m , and transform the variable x via $x = \bar{\psi}(t) = 2\psi(t/2)$. Thus,*

$$I[f] = \int_0^1 f(x) dx = \int_0^1 \bar{f}(t) dt;$$

$$\bar{f}(t) = f(\bar{\psi}(t))\bar{\psi}'(t) = f(2\psi(t/2))\psi'(t/2).$$

Let

$$\bar{Q}_n[f] = h \left[\sum_{i=1}^{n-1} \bar{f}(ih) + \frac{1}{2} \bar{f}(1) \right]; \quad h = \frac{1}{n}.$$

Then, whether $f'(0) \neq 0$ or not,

$$\bar{Q}_n[f] - I[f] = \begin{cases} O(h^{(j+1)(m+1)}) & \text{as } h \rightarrow 0, \text{ if } 2m \text{ odd integer,} \\ O(h^{2m+2}) & \text{as } h \rightarrow 0, \text{ otherwise.} \end{cases}$$

Thus, when $2m$ is an odd integer, $\bar{Q}_n[f] - I[f] = O(h^{3m+3})$ as $h \rightarrow 0$, at worst. In case $f'(0) = 0$, the result above can be refined as follows:

$$\bar{Q}_n[f] - I[f] = \begin{cases} O(h^{(j+2)(m+1)}) & \text{as } h \rightarrow 0, \text{ if } (j+1)(m+1) \text{ odd integer,} \\ O(h^{(j+1)(m+1)}) & \text{as } h \rightarrow 0, \text{ otherwise.} \end{cases}$$

Thus, in case $f'(0) = 0$, when $(j+1)(m+1)$ is an odd integer, $\bar{Q}_n[f] - I[f] = O(h^{4m+4})$ as $h \rightarrow 0$, at worst.

Note that, under the transformation $\bar{\psi}(t)$, the transformed abscissas $x_i = \bar{\psi}(i/n)$ are clustered in a small right neighborhood of $x = 0$; no clustering takes place near $x = 1$.

In connection with the use of $\bar{\psi}(t) = 2\psi(t/2)$ as the variable transformation in Theorem C.4, it is interesting to note that, under the condition that $f^{(2k+1)}(1) = 0$ for all $k \geq 0$, there is no contribution to the expansion of $\bar{Q}_n[f] - I[f]$ as $h \rightarrow 0$ from the endpoint $x = 1$. This is so for all values of m .

In case $f(0) \neq 0$ and $f(1) = 0$ in Theorem C.4, we write $I[f] = \int_0^1 g(x) dx$, with $g(x) = f(1 - x)$, and apply the method described there with $f(x)$ replaced by $g(x)$.

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