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Further extension of a class of periodizing variable transformations for numerical integration

Avram Sidi

Computer Science Department, Technion - Israel Institute of Technology, Haifa 32000, Israel

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Abstract

Class $\mathcal{S}_m$ variable transformations with integer m, for accurate numerical computation of finite-range integrals via the trapezoidal rule, were introduced and studied by the author. A representative of this class is the $\sin^m$-transformation. In a recent work of the author, this class was extended to arbitrary noninteger values of m, and it was shown that exceptionally high accuracies are achieved by the trapezoidal rule in different circumstances with suitable values of m. In another recent work by Monegato and Scuderi, the $\sin^m$-transformation was generalized by introducing two integers p and q, instead of the single integer m; we denote this generalization as the $\sin^{p,q}$-transformation here. When $p = q = m$, the $\sin^{p,q}$-transformation becomes the $\sin^m$-transformation. Unlike the $\sin^m$-transformation which is symmetric, the $\sin^{p,q}$-transformation is not symmetric when $p \neq q$, and this offers an advantage when the behavior of the integrand at one endpoint is quite different from that at the other endpoint. In view of the developments above, in the present work, we generalize the class $\mathcal{S}_m$ by introducing a new class of nonsymmetric variable transformations, which we denote as $\mathcal{S}_{p,q}$, where p and q can assume arbitrary noninteger values, such that the $\sin^{p,q}$-transformation is a representative of this class and $\mathcal{S}_m \subset \mathcal{S}_{m,m}$. We provide a detailed analysis of the trapezoidal rule approximation following a variable transformation from the class $\mathcal{S}_{p,q}$, and show that, with suitable and not necessarily integer p and q, it achieves an unusually high accuracy when the integrand has algebraic endpoint singularities. We also illustrate our results with numerical examples via the $\sin^{p,q}$-transformation. Finally, we discuss the computation of surface integrals in $\mathbb{R}^3$ containing point singularities with the help of class $\mathcal{S}_{p,q}$ transformations.

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1. Introduction

Consider the problem of evaluating finite-range integrals of the form

$$I[f] = \int_0^1 f(x)\mathrm{d}x, \tag{1.1}$$

E-mail address: asidi@cs.technion.ac.il.
URL: http://www.cs.technion.ac.il/~asidi/.

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where $f \in C^\infty(0,1)$ but is not necessarily continuous or differentiable at $x = 0$ and $x = 1$. $f(x)$ 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

$$I[f] = \int_0^1 \widehat{f}(t)\mathrm{d}t; \quad \widehat{f}(t) = f(\psi(t))\,\psi'(t), \tag{1.2}$$

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

$$\widehat{Q}_n[f] = h\left[\frac{1}{2}\widehat{f}(0) + \sum_{i=1}^{n-1}\widehat{f}(ih) + \frac{1}{2}\widehat{f}(1)\right]; \quad h = \frac{1}{n}. \tag{1.3}$$

[Normally, we also demand that $\psi(1-t) = 1-\psi(t)$, which forces on $\psi'(t)$ the symmetry property $\psi'(1-t) = \psi'(t)$.] If, in addition, $\psi(t)$ is chosen such that $\psi^{(i)}(0) = \psi^{(i)}(1) = 0$, $i = 1, 2, \ldots, p$, 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 $\widehat{f}(0) = \widehat{f}(1) = 0$, and $\widehat{Q}_n[f]$ becomes

$$\widehat{Q}_n[f] = h\sum_{i=1}^{n-1}\widehat{f}(ih). \tag{1.4}$$

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. Recently, they have also been used to improve the performance of the Gauss–Legendre quadrature. 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.)

In this paper, we concentrate on class $\mathcal{S}_m$ transformations of the author (see Sidi [9]), 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 and studied also in [9], has been used successfully in conjunction with lattice rules in multiple integration; see Sloan and Joe [17], Hill and Robinson [3], and Robinson and Hill [7]. The $\sin^m$-transformation has also been used in the computation of multi-dimensional integrals in conjunction with extrapolation methods by Verlinden, Potts, and Lyness [18]. (For a short list and discussion of the better known variable transformations, which we shall not repeat here, see [9].)

In a recent paper by the author, Sidi [14], the class $\mathcal{S}_m$ was extended by allowing m to take on arbitrary noninteger values. It was also shown in [14] that, for some special values of m chosen to depend on the behavior of $f(x)$ at $x = 0$ and $x = 1$, unusually high accuracies are attained by the trapezoidal rule in (1.4). This takes place, for example, when $f(0) = 0$ and $f(1) = 0$, and m is chosen such that $2m$ is an odd integer. These extended transformations have been used with success in the papers by Sidi [12,13,15] in the computation of integrals over smooth surfaces of bounded domains in $\mathbb{R}^3$ via the product trapezoidal rule.

Now, an extended class $\mathcal{S}_m$ variable transformation $\psi(t)$, with $m > 0$, has the property

$$\psi'(1-t) = \psi'(t), \qquad \psi(1-t) = 1 - \psi(t), \quad 0 \le t \le 1. \tag{1.5}$$

In words, $\psi'(t)$ is symmetric with respect to $t = 1/2$; hence $\psi(1/2) = 1/2$. In addition, $\psi(t)$ has the following asymptotic expansions as $t \to 0+$ and $t \to 1-$:

$$\begin{aligned}\psi'(t) &\sim \sum_{i=0}^{\infty}\epsilon_i t^{m+2i} \quad \text{as } t \to 0+,\\ \psi'(t) &\sim \sum_{i=0}^{\infty}\epsilon_i (1-t)^{m+2i} \quad \text{as } t \to 1-,\end{aligned} \tag{1.6}$$

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

$$
\begin{aligned}
\psi(t) &\sim \sum_{i=0}^{\infty} \epsilon_i \frac{t^{m+2i+1}}{m+2i+1} \quad \text{as } t \to 0+, \\
\psi(t) &\sim 1 - \sum_{i=0}^{\infty} \epsilon_i \frac{(1-t)^{m+2i+1}}{m+2i+1} \quad \text{as } t \to 1-.
\end{aligned}
\tag{1.7}
$$

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

The $\sin^m$-transformation of [14], a representative of the extended class $\mathcal{S}_m$, is given by

$$
\psi_m(t) = \frac{\int_0^t (\sin \pi u)^m \mathrm{d}u}{\int_0^1 (\sin \pi u)^m \mathrm{d}u}, \quad m > 0. \tag{1.8}
$$

In the case where m is an integer, which is the case considered originally in [9], the $\sin^m$-transformation $\psi_m(t)$ can be expressed as a finite combination of powers and trigonometric functions, and can be computed using the simple recursion relation

$$
\psi_m(t) = \psi_{m-2}(t) - \frac{\Gamma\left(\frac{m}{2}\right)}{2\sqrt{\pi}\,\Gamma\left(\frac{m+1}{2}\right)} (\sin \pi t)^{m-1} \cos \pi t,
$$

with the initial conditions

$$
\psi_0(t) = t \quad \text{and} \quad \psi_1(t) = \frac{1}{2}(1 - \cos \pi t) = \sin^2\left(\frac{\pi t}{2}\right).
$$

However, when m is not a integer, this is not possible; $\psi(t)$ has an infinite-series representation that converges quickly in this case. We refer the reader to [14] for details.

Now, in [14], we introduced the concept of *quality* of $\widehat{Q}_n[f]$ as follows: If $\psi(t) \sim \alpha t^q$ as $t \to 0+$ [hence $\psi(t) \sim 1 - \alpha(1-t)^q$ as $t \to 1-$], and if $\widehat{Q}_n[f] - I[f] = O(h^\sigma)$ as $h \to 0$, the quality of $\widehat{Q}_n[f]$ is the ratio σ/q. Note that the effective abscissas in $\widehat{Q}_n[f]$ given in (1.4) are $x_i \equiv \psi(ih) = \psi(i/n)$ and these cluster near $x = 0$ and $x = 1$ in the variable x and that the clustering increases with increasing q simultaneously with the accuracy of $\widehat{Q}_n[f]$. Because too much clustering is not desirable, we would like to get as much accuracy as possible from a given amount of clustering. In other words, we would like the quality of $\widehat{Q}_n[f]$ to be as high as possible. This is achieved by the variable transformations in $\mathcal{S}_m$ with special (not necessarily integer) values of m. For example, when $f(0) = f(1) = 0$ and $f'(0) \neq 0$ or $f'(1) \neq 0$, and $\psi \in \mathcal{S}_m$, the quality of $\widehat{Q}_n[f]$ is at least 3 if $2m$ is an odd integer; otherwise it is 2. When $f(0) = f(1) = 0$, $f''(0) = f''(1) = 0$, and $f'(0) \neq 0$ or $f'(1) \neq 0$, and $\psi \in \mathcal{S}_m$, the quality of $\widehat{Q}_n[f]$ is at least 4 if $2m$ is an odd integer; otherwise it is 2.

The $\sin^m$-transformation of [9] was generalized in a paper of Monegato and Scuderi [6]. This generalization, which we will denote as the $\sin^{p,q}$-transformation, is given as in

$$
\psi_{p,q}(t) = \frac{\Theta_{p,q}(t)}{\Theta_{p,q}(1)}; \quad \Theta_{p,q}(t) = \int_0^t \left(\sin \frac{1}{2}\pi u\right)^p \left(\cos \frac{1}{2}\pi u\right)^q \mathrm{d}u. \tag{1.9}
$$

Here, p and q are nonnegative integers, and this allows $\psi_{p,q}(t)$ to be computed via recursion relations, as has been shown in [6] and as we will discuss later in this work. Obviously, $\psi_{p,p}(t)$ (when $q = p$) is nothing but the $\sin^p$-transformation. (Note that the $\sin^m$-transformation is only one of the symmetric transformations generalized by Monegato and Scuderi in order to cope with integrands having integrable endpoint singularities of different strengths.) Finally, $\psi_{p,0}(t)$ (when $q = 0$) is simply $2\psi_p(t/2)$, $\psi_p(t)$ being the $\sin^p$-transformation defined in (1.8). The transformation $\psi_{p,0}(t)$, with integer p, has been used by Johnston [4], in conjunction with the Gauss–Legendre quadrature, for computing integrals with an integrable singularity at $x = 0$ only. It has also been used in [14, Theorem 4.4] in conjunction with the trapezoidal rule to treat the cases in which the integrand function $f(x)$ is such that $f^{(2k+1)}(1) = 0$, $k = 0, 1, \ldots$.

The purpose of the present work is to generalize the class $\mathcal{S}_m$ to what we will call the class $\mathcal{S}_{p,q}$, p and q being arbitrary numbers, not necessarily integers, and study the properties of the variable transformations in this class. In the next section, we introduce the class $\mathcal{S}_{p,q}$, and also show how functions in this class can be constructed. In addition, we show that the $\sin^{p,q}$-transformation in (1.9), with arbitrary p and q, belongs to $\mathcal{S}_{p,q}$. In Section 3, we show how the $\sin^{p,q}$-transformation with arbitrary p and q can be computed quickly and accurately. In Section 4, we study the behavior of the transformed trapezoidal rule $\widehat{Q}_n[f]$ when the variable transformation $\psi(t)$ is in $\mathcal{S}_{p,q}$. As part of this study, we also show how p and q can be chosen appropriately to "optimize" the quality of $\widehat{Q}_n[f]$ when $f(x)$ has algebraic endpoint singularities. That is, by choosing p and q appropriately, we are able to obtain high accuracy with a small amount of clustering of abscissas at the endpoints. In Section 5, we provide numerical examples, done with the $\sin^{p,q}$-transformation, that illustrate the theoretical results.

In Sections 6 and 7, we go back to numerical integration over surfaces of bounded sets in $\mathbb{R}^3$ in the presence of point singularities of the single-layer and double-layer types, and propose to use the variable transformations in the classes $\mathcal{S}_{p,q}$ with appropriate p and q.

Finally, in Section 8 we compare transformations in the class $\mathcal{S}_{p,q}$ with some new and analogous transformations that were presented in a recent paper by the author [16], and show that, in some cases, such as those treated in Section 6, the former have better convergence properties than the latter.

2. Generalization of the class $\mathcal{S}_m$: The class $\mathcal{S}_{p,q}$

We generalize the extended class $\mathcal{S}_m$, and define a new class of nonsymmetric variable transformations, which we will denote as $\mathcal{S}_{p,q}$, as follows:

Definition 2.1. A function $\psi(t)$ is in the class $\mathcal{S}_{p,q}$, with $p, q > 0$ but 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. $\psi'(t)$ has the following asymptotic expansions as $t \to 0+$ and $t \to 1-$:

$$\begin{aligned} \psi'(t) &\sim \sum_{i=0}^{\infty} \epsilon_i t^{p+2i} \quad \text{as } t \to 0+, \\ \psi'(t) &\sim \sum_{i=0}^{\infty} \delta_i (1-t)^{q+2i} \quad \text{as } t \to 1-, \end{aligned} \tag{2.1}$$

and $\epsilon_0, \delta_0 > 0$. Consequently,

$$\begin{aligned} \psi(t) &\sim \sum_{i=0}^{\infty} \epsilon_i \frac{t^{p+2i+1}}{p+2i+1} \quad \text{as } t \to 0+, \\ \psi(t) &\sim 1 - \sum_{i=0}^{\infty} \delta_i \frac{(1-t)^{q+2i+1}}{q+2i+1} \quad \text{as } t \to 1- . \end{aligned} \tag{2.2}$$

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

Remarks. 1. As in the case of the class $\mathcal{S}_m$ transformations, the fact that $\psi(t)$, as well as $\psi'(t)$, $\psi \in \mathcal{S}_{p,q}$, have the asymptotic expansions given in (2.1) and (2.2) – with consecutive powers of t and $(1-t)$ there increasing by 2 instead of by 1 – is the most important aspect of class $\mathcal{S}_{p,q}$ transformations. [Of course, we can replace the powers t^{p+2i} and $(1-t)^{q+2i}$ in (2.1) by t^{p+i} and $(1-t)^{q+i}$ and, thus, the powers t^{p+2i+1} and $(1-t)^{q+2i+1}$ in (2.2) by t^{p+i+1} and $(1-t)^{q+i+1}$ to obtain a larger class of variable transformations, even though these do not lead to results as good as those we obtain in this work. This is discussed in Section 8 in this work.]

2. Note that, unlike transformations in $\mathcal{S}_m$, transformations in $\mathcal{S}_{p,q}$ do not possess a symmetry property when $p \neq q$.
3. Also, if $\psi \in \mathcal{S}_{m,m}$ and $\psi'_{m,m}(t) = \psi'_{m,m}(1-t)$ [which also means that $\epsilon_i = \delta_i$, $i = 0, 1, \ldots$, in (2.1) and (2.2)], then $\psi \in \mathcal{S}_m$. In other words, $\mathcal{S}_m \subset \mathcal{S}_{m,m}$.

4. Finally, if $\psi \in \mathcal{S}_{p,q}$, and we define $\widetilde{\psi}(t) = 1 - \psi(1-t)$, then $\widetilde{\psi} \in \mathcal{S}_{q,p}$, because, by (2.2),

$$\begin{aligned} \widetilde{\psi}(t) &\sim 1 - \sum_{i=0}^{\infty} \epsilon_i \frac{(1-t)^{p+2i+1}}{p+2i+1} \quad \text{as } t \to 1-, \\ \widetilde{\psi}(t) &\sim \sum_{i=0}^{\infty} \delta_i \frac{t^{q+2i+1}}{q+2i+1} \quad \text{as } t \to 0+. \end{aligned} \tag{2.3}$$

Obviously, $\psi(t) + \widetilde{\psi}(1-t) = 1$ and $\psi'(t) = \widetilde{\psi}'(1-t)$, in addition.

2.1. Construction of functions in $\mathcal{S}_{p,q}$

We now show how functions in $\psi \in \mathcal{S}_{p,q}$ can be constructed. We claim that

$$\psi(t) = \frac{\int_0^t \omega'(u/2)\phi'((1-u)/2)\mathrm{d}u}{\int_0^1 \omega'(u/2)\phi'((1-u)/2)\mathrm{d}u} \in \mathcal{S}_{p,q} \quad \text{if} \quad \omega(t) \in \mathcal{S}_p \quad \text{and} \quad \phi(t) \in \mathcal{S}_q.$$

To see this, we need to verify that this $\psi(t)$ possesses all the properties mentioned in Definition 2.1. Of these, the first and third are seen to hold trivially. As for the second, it is sufficient to verify that one of the asymptotic expansions in (2.1) holds. We choose to verify the first, namely, that with $t \to 0+$. By the definition of the class $\mathcal{S}_m$, we have that

$$\omega'(t/2) \sim \sum_{i=0}^{\infty} \epsilon_i' t^{p+2i} \quad \text{as } t \to 0+;\ \epsilon_0 > 0.$$

Now, for any $\chi \in \mathcal{S}_m$, m being arbitrary, there holds $\chi^{(2i)}(1/2) = 0$, $i = 1, 2, \ldots$, as follows from (1.5). Therefore,

$$\phi'((1-t)/2) \sim \sum_{i=0}^{\infty} \epsilon_i'' t^{2i} \quad \text{as } t \to 0+;\ \epsilon_0'' > 0.$$

Multiplying these two asymptotic expansions, we see that $\psi'(t)$ has an asymptotic expansion as $t \to 0+$ of the form shown in (2.1).

Another way of generating transformations in $\mathcal{S}_{p,q}$ is as follows: Let $\alpha(t)$ and $\beta(t)$ be in $C^{\infty}[0, 1]$, with $\alpha(t) > 0$ and $\beta(t) > 0$ on $(0, 1)$, and have asymptotic expansions of the form

$$\alpha(t) \sim \sum_{i=0}^{\infty} \alpha_i' t^{2i+1} \quad \text{and} \quad \beta(t) \sim \sum_{i=0}^{\infty} \beta_i' t^{2i+1} \quad \text{as } t \to 0+, \tag{2.4}$$

and

$$\alpha(t) \sim \sum_{i=0}^{\infty} \alpha_i'' (1-t)^{2i} \quad \text{and} \quad \beta(t) \sim \sum_{i=0}^{\infty} \beta_i'' (1-t)^{2i} \quad \text{as } t \to 1-, \tag{2.5}$$

that can be differentiated term by term. Let also

$$\Theta_{p,q}(t) = \int_0^t [\alpha(u)]^p\, [\beta(1-u)]^q \,\mathrm{d}u. \tag{2.6}$$

Then

$$\psi(t) = \frac{\Theta_{p,q}(t)}{\Theta_{p,q}(1)} \in \mathcal{S}_{p,q}. \tag{2.7}$$

Making the substitution $u = 1 - v$ in the integral representation of $\Theta_{p,q}(t)$ in (2.6), we obtain

$$\Theta_{p,q}(t) = \int_{1-t}^{1} [\alpha(1-v)]^p [\beta(v)]^q \,\mathrm{d}v. \tag{2.8}$$

Thus, letting $t = 1$ in (2.6) and (2.8), we first obtain

$$c_{p,q} \equiv \Theta_{p,q}(1) = \Theta_{q,p}(1) \equiv c_{q,p} \quad \text{in case } \alpha(t) = \beta(t). \tag{2.9}$$

Rewriting (2.8) in the form

$$\Theta_{p,q}(t) = \int_0^1 [\alpha(1-v)]^p\,[\beta(v)]^q \mathrm{d}v - \int_0^{1-t} [\alpha(1-v)]^p\,[\beta(v)]^q \mathrm{d}v, \tag{2.10}$$

and invoking (2.9), we next have

$$\Theta_{p,q}(t) + \Theta_{q,p}(1-t) = c_{p,q} = c_{q,p} \quad \text{in case } \alpha(t) = \beta(t). \tag{2.11}$$

Functions in the class $\mathcal{S}_1$ can be used to construct $\alpha(t)$ and $\beta(t)$. If $\varpi(t)$ and $\varrho(t)$ are both in $\mathcal{S}_1$, then $\alpha(t)$ and $\beta(t)$, defined through $\alpha(t) = \varpi'(t/2)$ and $\beta(t) = \varrho'(t/2)$, satisfy (2.4) and (2.5) because $\chi^{(2i)}(1/2) = 0, i = 1, 2, \ldots,$ for any $\chi \in \mathcal{S}_m$, m being arbitrary, as follows from (1.5), and as mentioned above. Thus, $\psi(t)$ as defined in (2.6) and (2.7) is in $\mathcal{S}_{p,q}$. For example, choosing $\varpi(t)$ and $\varrho(t)$ to be both the $\sin^1$-transformation [that is, $\varpi(t) = \varrho(t) = \sin^2(\pi t/2)$], we have $\alpha(t) = \beta(t) = \frac{\pi}{2}\sin(\pi t/2)$; we thus obtain the $\sin^{p,q}$-transformation in (1.9), whose computation we treat in the next section.

3. The $\sin^{p,q}$-transformation

3.1. Computation with integer p and q

As mentioned earlier, the $\sin^{p,q}$-transformation [$\psi_{p,q}(t)$ in (1.9)] can be computed via recursion relations when p and q are integers. As shown in [6], by integration by parts, we have

$$\begin{aligned}
\Theta_{p,p}(t) &= -\frac{2^{-p}}{\pi p}(\sin \pi t)^{p-1}\cos \pi t + \frac{p-1}{4p}\,\Theta_{p-2,p-2}(t), \quad p \geq 2,\\
\Theta_{p,q}(t) &= \frac{2}{\pi(p+q)}\left(\sin\frac{\pi}{2}t\right)^{p+1}\left(\cos\frac{\pi}{2}t\right)^{q-1} + \frac{q-1}{p+q}\,\Theta_{p,q-2}(t), \quad p \geq 0,\ q \geq 2,\\
\Theta_{p,q}(t) &= -\frac{2}{\pi(p+q)}\left(\sin\frac{\pi}{2}t\right)^{p-1}\left(\cos\frac{\pi}{2}t\right)^{q+1} + \frac{p-1}{p+q}\,\Theta_{p-2,q}(t), \quad p \geq 2,\ q \geq 0,
\end{aligned}$$

with the starting values

$$\begin{aligned}
&\Theta_{0,0}(t) = t, \qquad \Theta_{1,0}(t) = \frac{2}{\pi}\left(1 - \cos\frac{\pi}{2}t\right),\\
&\Theta_{0,1}(t) = \frac{2}{\pi}\sin\frac{\pi}{2}t, \qquad \Theta_{1,1}(t) = \frac{1}{2\pi}(1 - \cos \pi t).
\end{aligned}$$

This completes the treatment of the case in which p and q are integers.

3.2. Computation with noninteger p or q

When p or q is not an integer, the recursion relations above cannot be used to compute $\psi_{p,q}(t)$ because the initial values are not known in simple terms. We proceed in a totally different way that is a generalization of that proposed and used in [14] for computing the extended $\sin^m$-transformation.

We propose to compute $\Theta_{p,q}(t)$ and $\Theta_{q,p}(t)$ simultaneously for $t \in [0, 1/2]$, and use the relation in (2.11) to compute them for $t \in [1/2, 1]$. The reason for this will become clear soon.

Denoting $c_{a,b} = \Theta_{a,b}(1)$, and recalling that $\alpha(t) = \beta(t) = \frac{\pi}{2}\sin(\pi t/2)$, we first note that $c_{p,q} = c_{q,p}$ by (2.9). Next, letting $t = 1/2$ in (2.11), we compute $\Theta_{p,q}(1) = c_{p,q}$ through

$$c_{p,q} = \Theta_{p,q}(1/2) + \Theta_{q,p}(1/2) = c_{q,p}.$$

We then compute $\psi_{p,q}(t)$ and $\psi_{q,p}(t)$ via

$$\psi_{p,q}(t) = \frac{\Theta_{p,q}(t)}{c_{p,q}} \quad \text{and} \quad \psi_{q,p}(t) = \frac{\Theta_{q,p}(t)}{c_{q,p}} \quad \text{for } t \in [0, 1/2],$$
$$\psi_{p,q}(t) = 1 - \psi_{q,p}(1-t) \quad \text{and} \quad \psi_{q,p}(t) = 1 - \psi_{p,q}(1-t) \quad \text{for } t \in [1/2, 1].$$

What remains is the computation of $\Theta_{p,q}(t)$ and $\Theta_{q,p}(t)$ for $t \in [0, 1/2]$. Of course, it is sufficient to consider one of them; we choose to consider $\Theta_{p,q}(t)$. In what follows, we derive two representations for $\Theta_{p,q}(t)$ in terms of the hypergeometric function $F(a, b; c; z)$, which has the series expansion

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

where $(x)_0 = 1$ and $(x)_k = x(x+1)\cdots(x+k-1)$ for $k = 1, 2, \ldots$. As we will see, both of these representations allow us the compute $\Theta_{p,q}(t)$ for $t \in [0, 1/2]$ (but not for $t \in [1/2, 1]$) in an efficient manner. Note also that the kth term in series representation of $F(a, b; c; z)$ is $O(k^{a+b-c-1}z^k)$ as $k \to \infty$, so that the series converges fast for small $|z| < 1$; its convergence slows down as $|z| \to 1$.

(i) Making the substitution $\xi = \sin(\pi u/2)$ in the integral representation of $\Theta_{p,q}(t)$, we obtain

$$\Theta_{p,q}(t) = \frac{2}{\pi} \int_0^S \xi^p \left(\sqrt{1-\xi^2}\right)^{q-1} \mathrm{d}\xi, \quad S = \sin\frac{\pi t}{2}.$$

Expanding the integrand about $\xi = 0$ and integrating the resulting (absolutely and uniformly convergent) series term by term, we obtain

$$\Theta_{p,q}(t) = \frac{2S^{p+1}}{\pi} \sum_{k=0}^{\infty} \frac{\left(\frac{1-q}{2}\right)_k}{k!} \frac{S^{2k}}{p+2k+1}, \quad S = \sin\frac{\pi t}{2}, \tag{3.1}$$

which can be expressed in terms of the hypergeometric function as in

$$\Theta_{p,q}(t) = \frac{2S^{p+1}}{\pi(p+1)} F\left(\frac{1}{2} - \frac{1}{2}q, \frac{1}{2}p + \frac{1}{2}; \frac{1}{2}p + \frac{3}{2}; S^2\right), \quad S = \sin\frac{\pi t}{2}. \tag{3.2}$$

For $k \geq \lfloor (q+1)/2 \rfloor$, the terms of this expansion are of the same sign and tend to zero as $k \to \infty$ essentially like $k^{-(q+3)/2}S^{2k}$, and hence, by the fact that $0 \leq S \leq \sin(\pi/4) = 1/\sqrt{2}$, at worst like $k^{-(q+3)/2}2^{-k}$. Thus, the expansion above converges quickly and can be used for the actual computation of $\Theta_{p,q}(t)$. For example, double-precision accuracy (approximately 14 decimal digits) can be achieved for $\Theta_{p,q}(t)$ with $p = 0.5$ and $q = 0.1$ and $t = 0.005, 0.05, 0.1, 0.2, 0.3, 0.4, 0.5$ by direct summation of the first 3, 5, 7, 11, 17, 24, 38 terms, respectively, of the series in (3.1).

Furthermore, we can also use a nonlinear sequence transformation, such as that of Shanks [8] (or the equivalent ϵ-algorithm of Wynn [19]) or of Levin [5], to accelerate the convergence of this expansion. Both transformations are treated in detail in the recent book by Sidi [10].

(ii) Invoking in (3.2) one of the so-called linear transformation formulas, see Abramowitz and Stegun [1, p. 559, formulas 15.3.4 and 15.3.5], and using the fact $\frac{S^2}{S^2-1} = -\tan^2\frac{\pi t}{2}$, and the relations

$$\sin x = \frac{\tan x}{\sqrt{1+\tan^2 x}} \quad \text{and} \quad \cos x = \frac{1}{\sqrt{1+\tan^2 x}}, \quad 0 \leq x \leq \frac{\pi}{2},$$

we obtain

$$\Theta_{p,q}(t) = \frac{2T^{p+1}}{\pi(p+1)(1+T^2)^{(p+q)/2}} F\left(1, \frac{1}{2} - \frac{1}{2}q; \frac{1}{2}p + \frac{3}{2}; -T^2\right), \quad T = \tan\frac{\pi t}{2} \tag{3.3}$$

which has the expansion

$$\Theta_{p,q}(t) = \frac{2T^{p+1}}{\pi(p+1)(1+T^2)^{(p+q)/2}} \sum_{k=0}^{\infty} \frac{\left(\frac{1}{2} - \frac{1}{2}q\right)_k}{\left(\frac{1}{2}p + \frac{3}{2}\right)_k} (-T^2)^k; \quad T = \tan\frac{\pi t}{2}. \tag{3.4}$$

Since $0 < T \le \tan(\pi/4) = 1$ for $0 \le t \le 1/2$, the terms of this series tend to zero like $k^{-1-(p+q)/2}T^{2k}$ as $k \to \infty$. Consequently, this expansion converges very slowly for t close to 1/2 because $T^2 \to 1$ as $t \to 1/2$. However, it is an essentially alternating series because, for $k \ge \lfloor (q+1)/2 \rfloor$, its terms alternate in sign. This being the case, the series in (3.4) turns out to be ideal for the actual computation of $\Theta_{p,q}(t)$ because 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.

Summary of computation of $\psi_{p,q}(t)$

We now summarize the steps by which one can compute $\psi_{p,q}(t)$ for $t \in [0, 1]$ to machine accuracy quickly and efficiently. Clearly, before everything else, one must have a code for computing $\Theta_{a,b}(t)$, via

$$\Theta_{a,b}(t) = \frac{2S^{a+1}}{\pi} \sum_{k=0}^{\infty} \frac{\left(\frac{1-b}{2}\right)_k}{k!} \frac{S^{2k}}{a+2k+1}, \quad S = \sin\frac{\pi t}{2}.$$

Recall that the series here converges quickly for $t \in [0, 1/2]$ and its convergence can be monitored easily since its terms are ultimately of the same sign. In addition, by letting $h_k = (\frac{1-b}{2})_k S^{2k}/k!$, and observing that $h_{k+1} = (\frac{1-b}{2} + k)S^2/(k+1)$, the cost of computing each term of the series is reduced to just a few arithmetic operations, once S has been computed. Finally, the number of terms of the series required for computing its sum to machine accuracy becomes smaller as t becomes smaller.

1. Compute $\Theta_{p,q}(1/2)$ and $\Theta_{q,p}(1/2)$, and set $c_{p,q} = c_{q,p} = \Theta_{p,q}(1/2) + \Theta_{q,p}(1/2)$.
2. For $t \in [0, 1/2]$, compute $\Theta_{p,q}(t)$ and $\Theta_{q,p}(t)$, and set $\psi_{p,q}(t) = \Theta_{p,q}(t)/c_{p,q}$ and $\psi_{q,p}(t) = \Theta_{q,p}(t)/c_{q,p}$.
3. For $t \in [1/2, 1]$, compute $\psi_{p,q}(t)$ via $\psi_{p,q}(t) = 1 - \psi_{q,p}(1-t)$.

4. Analysis of the trapezoidal rule with class $\mathcal{S}_{p,q}$ transformations

In this section, we analyze the behavior of the transformed trapezoidal rule $\widehat{Q}_n[f]$ given in (1.4) for when the integrand $f(x)$ is infinitely differentiable in (0, 1) and possibly has algebraic singularities at $x = 0$ and/or $x = 1$.

Euler–Maclaurin expansions concerning the trapezoidal rule approximations of finite-range integrals $\int_a^b u(x)\mathrm{d}x$ are the main analytical tool that we use in our study. For the sake of easy reference, we reproduce here the relevant Euler–Maclaurin expansion due to the author (see Sidi [11, Corollary 2.2]) as Theorem 4.1. This theorem is a special case of another very general theorem from [11], and is expressed in terms of the asymptotic expansions of $u(x)$ as $x \to a+$ and $x \to b-$ and is easy to write down and use.

Theorem 4.1. *Let $u \in C^\infty(a, b)$, and assume that $u(x)$ has the asymptotic expansions*

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

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

where the γ_s and δ_s are distinct complex numbers that satisfy

$$-1 < \Re\gamma_0 \le \Re\gamma_1 \le \Re\gamma_2 \le \cdots; \quad \lim_{s\to\infty} \Re\gamma_s = +\infty,$$

$$-1 < \Re\delta_0 \le \Re\delta_1 \le \Re\delta_2 \le \cdots; \quad \lim_{s\to\infty} \Re\delta_s = +\infty.$$

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

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

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

It is clear from Theorem 4.1 that positive even powers of $(x-a)$ and $(b-x)$, if present in the asymptotic expansions of $u(x)$ as $x \to a+$ and $x \to b-$, do not contribute to the asymptotic expansion of $h\sum_{i=1}^{n-1} u(a+ih)$ as $h \to 0$.

In addition, if γ_p is the first of the γ_s that is different from $2, 4, 6, \ldots$, and if δ_q is the first of the δ_s that is different from $2, 4, 6, \ldots$, then

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

Here is our main result:

Theorem 4.2. *Let $f \in C^\infty(0,1)$, and assume that $f(x)$ has the asymptotic expansions*

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

Here γ_s and δ_s are distinct complex numbers that satisfy

$$-1 < \Re\gamma_0 \le \Re\gamma_1 \le \Re\gamma_2 \le \cdots; \qquad \lim_{s\to\infty} \Re\gamma_s = +\infty,$$
$$-1 < \Re\delta_0 \le \Re\delta_1 \le \Re\delta_2 \le \cdots; \qquad \lim_{s\to\infty} \Re\delta_s = +\infty.$$

Assume furthermore that, for each positive integer k, $f^{(k)}(x)$ has asymptotic expansions as $x \to 0+$ and $x \to 1-$ that are obtained by differentiating those of $f(x)$ term by term k times. Let $I[f] = \int_0^1 f(x)\mathrm{d}x$, and let us now make the transformation of variable $x = \psi(t)$, where $\psi \in \mathcal{S}_{p,q}$, 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 $h = 1/n$, $n = 1, 2, \ldots$. Then the following hold:

(i) *In the worst case,*

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

(ii) *If γ_0 and δ_0 are real, and if $p = (2k-\gamma_0)/(\gamma_0+1)$ and $q = (2l-\delta_0)/(\delta_0+1)$, where k and l are positive integers, then*

$$\widehat{Q}_n[f] - I[f] = O\left(h^\omega\right) \quad \text{as } h \to 0; \quad \omega = \min\{(\Re\gamma_1 + 1)(p+1), (\Re\delta_1 + 1)(q+1)\},$$

at worst.

Remark. If $f(x) = x^\mu(1-x)^\nu g(x)$, $g(x)$ being infinitely differentiable on $[0,1]$, then $f(x)$ satisfies the conditions of the theorem. In such a case, if $f(x)$ has full Taylor series at $x=0$ and $x=1$, we have $\gamma_s = \mu + s$ and $\delta_s = \nu + s$, $s = 0, 1, \ldots$. Note that this $f(x)$ has an algebraic branch singularity at $x=0$ if μ is not a positive integer. Similarly, it has an algebraic branch singularity at $x=1$ if ν is not a positive integer.

Proof. It is clear from Theorem 4.1 that we need to analyze the asymptotic expansions of the transformed integrand $\widehat{f}(t) = f(\psi(t))\,\psi'(t)$ as $t \to 0$ and $t \to 1$. To proceed with this analysis, we need the following: Let $w(\xi)$ denote generically any function that has an asymptotic expansion of the form $\sum_{i=0}^\infty w_i\xi^{2i}$ as $\xi \to 0+$. Then

$$g_i(\xi) = \xi^{r_i} w(\xi), \quad i = 1, \ldots, k, \quad \Rightarrow \quad \prod_{i=1}^{k} g_i(\xi) = \xi^r w(\xi), \quad r = \sum_{i=1}^{k} r_i.$$

Because $\psi(t) \to 0$ as $t \to 0$ and $\psi(t) \to 1$ as $t \to 1$, we first have

$$\widehat{f}(t) \sim \sum_{s=0}^{\infty} c_s[\psi(t)]^{\gamma_s}\psi'(t) \quad \text{as } t \to 0; \qquad \widehat{f}(t) \sim \sum_{s=0}^{\infty} d_s[1-\psi(t)]^{\delta_s}\psi'(t) \quad \text{as } t \to 1.$$

Invoking (2.1) and (2.2), and re-expanding these asymptotic series, we have that the sth term in the first of these series contributes the sum

$$K_s^{(0)}(t) := \sum_{i=0}^{\infty} e_{si}^{(0)} t^{\gamma_s(p+1)+p+2i} \quad \text{as } t \to 0; \qquad e_{s0}^{(0)} = c_s\epsilon_0^{\gamma_s+1}/(p+1)^{\gamma_s} \neq 0, \tag{4.1}$$

whereas the sth term in the second series contributes the sum

$$K_s^{(1)}(t) := \sum_{i=0}^{\infty} e_{si}^{(1)}(1-t)^{\delta_s(q+1)+q+2i} \quad \text{as } t \to 1; \qquad e_{s0}^{(1)} = d_s\epsilon_0^{\delta_s+1}/(q+1)^{\delta_s} \neq 0. \tag{4.2}$$

Thus, by Theorem 4.1, the most dominant terms in the expansion of $\widehat{Q}_n[f] - I[f]$ as $h \to 0$ are $e_{00}^{(0)}h^{(\gamma_0+1)(p+1)}$ coming from the endpoint $x = 0$, and $e_{00}^{(1)}h^{(\delta_0+1)(q+1)}$ coming from the endpoint $x = 1$. This proves part (i) of the theorem.

To prove part (ii), we note from Theorem 4.1 that if we choose p such that $\gamma_s(p+1)+p$ is a positive even integer, then *all* the powers of t in the asymptotic expansion $K_s^{(0)}(t)$ of (4.1) are also even, and hence do not contribute to the asymptotic expansion of $\widehat{Q}_n[f] - I[f]$. Similarly, if we choose q such that $\delta_s(q+1)+q$ is a positive even integer, then *all* the powers of $(1-t)$ in the asymptotic expansion $K_s^{(1)}(t)$ of (4.2) are also even, and hence do not contribute to the asymptotic expansion of $\widehat{Q}_n[f]-I[f]$. Thus, when γ_0 and δ_0 are real, if we choose p and q such that $\gamma_0(p+1)+p = 2k$ and $\delta_0(q+1)+q = 2l$, where k and l are positive integers, then neither $K_0^{(0)}(t)$ in (4.1) nor $K_0^{(1)}(t)$ in (4.2) contributes to the asymptotic expansion of $\widehat{Q}_n[f] - I[f]$. The largest terms that possibly contribute are (i) $e_{10}^{(0)}t^{\gamma_1(p+1)+p}$, the first term of $K_1^{(0)}(t)$, provided $\gamma_1(p+1)+p$ is not an even integer, and (ii) $e_{10}^{(1)}(1-t)^{\delta_1(q+1)+q}$, the first term of $K_1^{(1)}(t)$, provided $\delta_1(q+1)+q$ is not an even integer. Under these conditions, the contributions of these terms to $\widehat{Q}_n[f]-I[f]$ are $E^{(0)}h^{(\gamma_1+1)(p+1)}$ and $E^{(1)}h^{(\delta_1+1)(q+1)}$, respectively, $E^{(0)}$, $E^{(1)}$ being some constants. This proves the result in part (ii). ■

Remark. Note that the result in part (ii) of Theorem 4.2 is made possible by our definition of the class $\mathcal{S}_{p,q}$ transformations, where we have excluded the powers $t^{p+1}, t^{p+3}, \ldots,$ and $(1-t)^{q+1}, (1-t)^{q+3}, \ldots,$ from the asymptotic expansions of $\psi'(t)$ as $t \to 0+$ and $t \to 1-$.

Corollary 4.3. *In the case of* $f(x) = x^\mu(1-x)^\nu g(x)$, $g(x)$ *being infinitely differentiable on* $[0,1]$, *then the following hold:*

(i) *In the worst case,*

$$\widehat{Q}_n[f] - I[f] = O\left(h^\omega\right) \quad \text{as } h \to 0;\ \omega \geq \min\{(\Re\mu+1)(p+1), (\Re\nu+1)(q+1)\}.$$

(ii) *If* μ *and* ν *are real, and if* $p = (2k-\mu)/(\mu+1)$ *and* $q = (2l-\nu)/(\nu+1)$, *where* k *and* l *are positive integers, then*

$$\widehat{Q}_n[f] - I[f] = O\left(h^\omega\right) \quad \text{as } h \to 0;\ \omega \geq \min\{(\mu+2)(p+1), (\nu+2)(q+1)\}.$$

When $\mu = \nu = c$ in part (ii) of Corollary 4.3, we can use a class $\mathcal{S}_m$ variable transformation with $m = (2k-c)/(c+1)$ to obtain the optimal result $\widehat{Q}_n[f] - I[f] = O(h^\omega)$ as $h \to 0$, where $\omega \geq (c+2)(m+1)$.

When $\mu \neq \nu$ in part (ii) of Corollary 4.3, we choose the integers k and l such that $(\mu+2)(p+1) \approx (\nu+2)(q+1)$, that is,

$$\frac{2k+1}{2l+1} \approx \frac{\nu+2}{\nu+1} \cdot \frac{\mu+1}{\mu+2}.$$

(Thus, by choosing k first, we can determine l, and vice versa.) This guarantees that the singularities of the transformed integrand $\widehat{f}(t) = f(\psi(t))\psi'(t)$ at the endpoints are of approximately the same strength.

5. Numerical examples

In this section, we provide two examples to illustrate the validity of the results of the preceding section. The computations for these examples were done in quadruple-precision arithmetic (approximately 35 decimal digits).

Example 5.1. Consider the integral

$$\int_0^1 x^\mu \mathrm{d}x = \frac{1}{1+\mu}, \quad \mu > -1.$$

Table 1
Errors in the rules $\widehat{Q}_n[f]$ for the integral of Example 5.1 obtained with $n = 2^k$, $k = 1(1)10$, and with the $\sin^{p,q}$-transformation

n	$j = 1$	$j = 2$	$j = 3$	$j = 4$	$j = 5$	$j = 6$	$j = 7$	$j = 8$	$j = 9$	$j = 10$
2	1.81D−02	1.50D−03	3.22D−01	3.36D−01	5.91D−01	6.03D−01	8.21D−01	8.31D−01	1.02D+00	1.03D+00
4	2.17D−03	1.46D−05	5.66D−04	4.72D−07	1.77D−04	5.28D−04	2.74D−02	2.94D−02	7.70D−02	7.99D−02
8	2.83D−04	1.82D−07	1.51D−05	1.23D−08	2.28D−06	3.00D−08	5.46D−07	2.31D−07	7.49D−07	1.95D−07
16	3.76D−05	2.68D−09	4.79D−07	7.85D−12	1.63D−08	1.47D−13	1.06D−09	4.06D−15	1.13D−10	3.57D−13
32	5.03D−06	4.12D−11	1.58D−08	7.03D−15	1.32D−10	6.87D−18	2.03D−12	2.32D−20	5.03D−14	2.09D−22
64	6.73D−07	6.42D−13	5.28D−10	6.72D−18	1.09D−12	3.93D−22	4.17D−15	7.67D−26	2.53D−17	3.79D−29
128	9.01D−08	1.00D−14	1.77D−11	6.53D−21	9.12D−15	2.36D−26	8.68D−18	2.83D−31	1.31D−20	9.53D−34
256	1.21D−08	1.57D−16	5.92D−13	6.37D−24	7.63D−17	1.44D−30	1.81D−20	4.24D−34	6.84D−24	9.53D−34
512	1.62D−09	2.45D−18	1.98D−14	6.22D−27	6.39D−19	1.06D−34	3.80D−23	5.30D−34	3.58D−27	1.91D−33
1024	2.17D−10	3.82D−20	6.64D−16	6.07D−30	5.35D−21	4.24D−34	7.94D−26	1.06D−33	1.87D−30	4.24D−34

In column j, we have chosen $p = (j + 0.9 - \mu)/(1 + \mu)$ and $q = j + 0.9$ when j is odd, while $p = (j - \mu)/(1 + \mu)$ and $q = j$ when j is even.

In this case, we have

$$f(x) = x^{\mu} \quad \text{and} \quad f(x) = \sum_{s=0}^{\infty} (-1)^s \binom{\mu}{s} (1 - x)^s.$$

Of these, the first is a single-term series representing $f(x)$ asymptotically as $x \to 0+$ with $\gamma_0 = \mu$, while the second is a (convergent) series representing $f(x)$ asymptotically as $x \to 1-$ with $\delta_s = s$, $s = 0, 1, \ldots$. (Note that, in the notation of Corollary 4.3, $\nu = 0$ now.) Thus, if we choose p and q arbitrarily, we will obtain, by part (i) of Theorem 4.2 and Corollary 4.3,

$$\widehat{Q}_n[f] - I[f] = O\left(h^{\omega}\right) \quad \text{as } h \to 0; \quad \omega = \min\{(\mu + 1)(p + 1), (q + 1)\}.$$

In the case of $p = (2k - \mu)/(1 + \mu)$ and $q = 2l$, with k, l positive integers, we will obtain, by part (ii) of Theorem 4.2,

$$\widehat{Q}_n[f] - I[f] = O\left(h^{\omega}\right) \quad \text{as } h \to 0; \quad \omega = 2(q + 1).$$

This is so because the asymptotic expansion of $f(x)$ as $x \to 0+$ consists of only the term x^{μ}.

In our computations, we have taken $\mu = 0.1$.

In Table 1, we give the relative errors in the $\widehat{Q}_n[f]$ for $n = 2^k$, $k = 1, \ldots, 10$, obtained with the $\sin^{p,q}$-transformation. In column j of this table, we have chosen $p = (j + 0.9 - \mu)/(1 + \mu)$ and $q = (j + 0.9 - \nu)/(1 + \nu)$ when j is odd, while $p = (j - \mu)/(1 + \mu)$ and $q = (j - \nu)/(1 + \nu)$ when j is even. The superior convergence of the columns with j an even integer is clearly demonstrated. [Note that the p (the q), hence the clusterings of the effective abscissas $x_i = \psi(i/n)$ near $x = 0$ (near $x = 1$) with $j = 2k - 1$ and $j = 2k$ are approximately the same for each k.]

In Table 2, we give the numbers

$$\rho_{p,q,k} = \frac{1}{\log 2} \cdot \log \left(\frac{|\widehat{Q}_{2^k}[f] - I[f]|}{|\widehat{Q}_{2^{k+1}}[f] - I[f]|} \right),$$

for the same values of p and q and for $k = 1, 2, \ldots, 9$. It is seen that, with increasing k, the $\rho_{p,q,k}$ are tending to $\min\{(\mu + 1)(p + 1), (q + 1)\}$ when j an odd integer, and to $2(q + 1)$ when j is an even integer, completely in accordance with Theorem 4.2 and Corollary 4.3. (With the floating-point arithmetic we are using, this convergence seems to be less visible for relatively large p and q in the columns with even j.)

Example 5.2. Consider the integral

$$\int_0^1 f(x) = 0, \quad f(x) = \frac{\mathrm{d}}{\mathrm{d}x} \left[x^{\mu+1} (1 - x)^{\nu+1} w(x) \right], \quad \mu, \nu > 0, \; w \in C^{\infty}[0, 1].$$

In this case, we have

$$f(x) = x^{\mu} (1 - x)^{\nu} g(x),$$

where

$$g(x) = [(\mu + 1)(1 - x) - (\nu + 1)x]\, w(x) + x(1 - x) w'(x).$$

Table 2

The numbers $\rho_{p,q,k} = \frac{1}{\log 2} \cdot \log \left(\frac{|\widehat{Q}_{2^k}[f]-I[f]|}{|\widehat{Q}_{2^{k+1}}[f]-I[f]|} \right)$, with p, q, $f(x)$, and $\widehat{Q}_n[f]$ as in Table 1, for $k = 1(1)9$

n	$j=1$	$j=2$	$j=3$	$j=4$	$j=5$	$j=6$	$j=7$	$j=8$	$j=9$	$j=10$
1	3.058	6.682	9.152	19.444	11.709	10.157	4.906	4.821	3.732	3.692
2	2.943	6.330	5.227	5.262	6.274	14.106	15.613	16.956	16.651	18.646
3	2.912	6.086	4.979	10.614	7.124	17.640	9.009	25.763	12.693	19.060
4	2.903	6.021	4.919	10.125	6.957	14.382	9.026	17.417	11.134	30.666
5	2.901	6.005	4.905	10.031	6.914	14.092	8.931	18.207	10.958	22.395
6	2.900	6.001	4.901	10.008	6.903	14.023	8.908	18.049	10.914	15.281
7	2.900	6.000	4.900	10.002	6.901	14.005	8.902	9.382	10.904	0.000
8	2.900	6.000	4.900	10.000	6.900	13.729	8.900	−0.322	10.901	−1.000
9	2.900	6.000	4.900	10.000	6.900	−2.000	8.900	−1.000	10.900	2.170
∞	2.9	6	4.9	10	6.9	14	8.9	18	10.9	22

Table 3

Errors in the rules $\widehat{Q}_n[f]$ for the integral of Example 5.2, obtained with $n = 2^k$, $k = 1(1)10$, and with the $\sin^{p,q}$-transformation

n	$j=1$	$j=2$	$j=3$	$j=4$	$j=5$	$j=6$	$j=7$	$j=8$	$j=9$	$j=10$
2	4.59D−02	4.58D−02	3.55D−02	3.46D−02	1.44D−02	1.32D−02	1.27D−02	1.42D−02	4.38D−02	4.54D−02
4	3.92D−04	6.34D−04	5.13D−03	5.55D−03	8.66D−03	8.53D−03	1.05D−03	4.44D−04	1.38D−02	1.47D−02
8	2.02D−05	5.11D−06	8.31D−07	7.95D−07	6.78D−06	5.76D−06	1.11D−04	1.24D−04	4.73D−04	4.95D−04
16	3.43D−06	8.24D−08	9.68D−09	5.79D−10	9.89D−10	2.01D−11	4.24D−10	3.01D−10	3.53D−09	4.24D−09
32	4.75D−07	1.31D−09	3.13D−10	1.16D−12	7.40D−12	3.19D−15	2.69D−13	1.21D−17	1.06D−14	4.36D−19
64	6.39D−08	1.83D−11	1.05D−11	2.63D−15	6.05D−14	7.16D−19	5.45D−16	2.42D−22	5.24D−18	1.06D−25
128	8.57D−09	1.65D−13	3.53D−13	6.41D−18	5.04D−16	1.70D−22	1.13D−18	5.31D−27	2.70D−21	2.12D−31
256	1.15D−09	1.96D−15	1.18D−14	1.62D−20	4.21D−18	4.12D−26	2.36D−21	1.19D−31	1.41D−24	9.91D−36
512	1.54D−10	1.81D−16	3.96D−16	4.17D−23	3.53D−20	1.00D−29	4.95D−24	3.74D−35	7.37D−28	4.26D−35
1024	2.06D−11	7.47D−18	1.33D−17	1.08D−25	2.95D−22	2.42D−33	1.04D−26	1.11D−34	3.86D−31	2.53D−35

In column j, we have chosen $p = (j + 0.9 - \mu)/(1 + \mu)$ and $q = (j + 0.9 - \nu)/(1 + \nu)$ when j is odd, while $p = (j - \mu)/(1 + \mu)$ and $q = (j - \nu)/(1 + \nu)$ when j is even.

If $w(0)$ and $w(1)$ are both nonzero, we have that $g(0)$ and $g(1)$ are both nonzero as well, and this implies that $\gamma_0 = \mu$ and $\delta_0 = \nu$. Thus, if we choose p and q arbitrarily, we will obtain, by part (i) of Theorem 4.2 and Corollary 4.3,

$$\widehat{Q}_n[f] - I[f] = O\left(h^{\omega}\right) \quad \text{as } h \to 0; \ \omega = \min\{(\mu+1)(p+1), (\nu+1)(q+1)\}.$$

In the case of $p = (2k - \mu)/(1 + \mu)$ and $q = (2l - \nu)/(1 + \nu)$, with k, l positive integers, we will obtain, by part (ii) of Theorem 4.2 and Corollary 4.3,

$$\widehat{Q}_n[f] - I[f] = O\left(h^{\omega}\right) \quad \text{as } h \to 0, \ \omega = \min\{(\mu+2)(p+1), (\nu+2)(q+1)\}.$$

In our computations, we have taken $\mu = 0.1$ and $\nu = 0.4$ and $w(x) = 1/(1 + x)$.

In Table 3, we give the absolute errors (recall that $I[f] = 0$) in the $\widehat{Q}_n[f]$ for $n = 2^k$, $k = 1, \ldots, 10$, obtained with the $\sin^{p,q}$-transformation. In column j of this table, we have chosen $p = (j + 0.9 - \mu)/(1 + \mu)$ and $q = (j + 0.9 - \nu)/(1 + \nu)$ when j is odd, while $p = (j - \mu)/(1 + \mu)$ and $q = (j - \nu)/(1 + \nu)$ when j is even. The superior convergence of the columns with j an even integer is again clearly demonstrated. [Note that the p (the q), and hence the clusterings of the effective abscissas $x_i = \psi(i/n)$ near $x = 0$ (near $x = 1$) with $j = 2k - 1$ and $j = 2k$, are approximately the same for each k.]

In Table 4, we give the numbers $\rho_{p,q,k}$ defined in the preceding example for the same values of p and q and for $k = 1, 2, \ldots, 9$. It is seen that, with increasing k, the $\rho_{p,q,k}$ are tending to $\min\{(\mu + 1)(p + 1), (\nu + 1)(q + 1)\}$ when j an odd integer, and to $\min\{(\mu + 2)(p + 1), (\nu + 2)(q + 1)\}$ when j is an even integer, completely in accordance with Theorem 4.2 and Corollary 4.3. (As in the preceding example, with the floating-point arithmetic we are using, this convergence seems to be less visible for relatively large p and q in the columns with even j.)

Table 4

The numbers $\rho_{p,q,k} = \frac{1}{\log 2} \cdot \log \left(\frac{|\widehat{Q}_{2^k}[f]-I[f]|}{|\widehat{Q}_{2^{k+1}}[f]-I[f]|} \right)$, with $p, q, f(x)$, and $\widehat{Q}_n[f]$ as in Table 3, for $k = 1(1)9$

k	$j=1$	$j=2$	$j=3$	$j=4$	$j=5$	$j=6$	$j=7$	$j=8$	$j=9$	$j=10$
1	6.871	6.175	2.788	2.640	0.733	0.626	3.593	4.998	1.662	1.628
2	4.279	6.955	12.593	12.771	10.319	10.531	3.250	1.846	4.869	4.892
3	2.557	5.954	6.424	10.422	12.743	18.132	17.997	18.647	17.031	16.833
4	2.854	5.977	4.952	8.970	7.062	12.618	10.620	24.568	18.352	33.178
5	2.893	6.162	4.894	8.778	6.933	12.121	8.948	15.611	10.978	21.974
6	2.899	6.789	4.897	8.681	6.908	12.038	8.912	15.475	10.919	18.932
7	2.900	6.398	4.899	8.629	6.902	12.012	8.903	15.440	10.905	14.382
8	2.900	3.439	4.900	8.601	6.901	12.004	8.901	11.640	10.901	−2.104
9	2.900	4.595	4.900	8.587	6.900	12.017	8.900	−1.565	10.900	0.751
∞	2.9	4.971···	4.9	8.4	6.9	12	8.9	15.257···	10.9	18.857···

6. $\mathcal{S}_{p,q}$ transformations and numerical integration of singular functions over smooth surfaces in $\mathbb{R}^3$

In [12,15], we considered the numerical evaluation of integrals with point singularities of the single-layer and double-layer types over surfaces of bounded sets in $\mathbb{R}^3$ with the help of class $\mathcal{S}_m$ variable transformations. We consider this problem here again in view of the new transformations that we have developed.

Let the integral in question be

$$I[f] = \iint_S f(Q)\mathrm{d}A_S, \quad Q \in S, \tag{6.1}$$

where S is the surface of a closed and bounded set in $\mathbb{R}^3$ and $\mathrm{d}A_S$ is the corresponding surface area element. We assume that the surface S is infinitely smooth and homeomorphic to U, the surface of the unit sphere, and that the Jacobian matrix of the corresponding mapping from U to S is nonsingular. The integrand $f(Q)$ is assumed to be smooth over S, except for a point singularity of the single-layer or double-layer type, say, at the point $P \in S$.

To compute $I[f]$ numerically, we first map U to S. Next, we rotate the coordinate system on U such that either the north pole or the south pole of U is mapped to P on S; this we do through an orthogonal transformation such as the Householder transformation. Following that, we express the transformed integral in terms of the standard spherical coordinates θ and ϕ, $0 \le \theta \le \pi$, $0 \le \phi \le 2\pi$. Let us denote the resulting integral in the form

$$I[f] = \int_0^{\pi} \left[\int_0^{2\pi} F(\theta,\phi)\mathrm{d}\phi \right] \mathrm{d}\theta. \tag{6.2}$$

We next transform the variable θ via $\theta = \Psi(t)$. In [12,15], $\Psi(t)$ was chosen to be related to a transformation in the class $\mathcal{S}_m$ for some m. We now take it to be a constant multiple of a transformation in $\mathcal{S}_{p,q}$ for some suitable $p > 0$ and $q > 0$. Specifically, we choose

$$\Psi(t) = \begin{cases} \pi\,\psi_{m,2l}(t) & \text{if singularity at south pole} \\ \pi\,\psi_{2l,m}(t) & \text{if singularity at north pole;} \end{cases} \qquad m > 0, \quad l = 1, 2, \ldots. \tag{6.3}$$

The transformed integral is

$$I[f] = \int_0^1 \left[\int_0^{2\pi} \widehat{F}(t,\phi)\mathrm{d}\phi \right] \mathrm{d}t; \qquad \widehat{F}(t,\phi) = F\left(\Psi(t),\phi\right)\, \Psi'(t). \tag{6.4}$$

Finally, we approximate $I[f]$ by the product trapezoidal rule defined as follows:

$$\widehat{T}_{n,n'}[f] = hh' \sum_{j=1}^{n-1} \sum_{i=1}^{n'} \widehat{F}(jh, ih'); \qquad h = \frac{1}{n},\ h' = \frac{2\pi}{n'}. \tag{6.5}$$

Note that, with $\Psi(t)$ as in (6.3), there holds $\Psi'(0) = \Psi'(1) = 0$. As a result, we have $\widehat{F}(0, \phi) = \widehat{F}(1, \phi) = 0$, and this explains why the summation over j in $\widehat{T}_{n,n'}[f]$ does not contain the terms with $j = 0$ and $j = n$. Now, one of these terms comes from the mapping of the point of singularity and is not immediately available if it is nonzero, in which case it is defined as a limit; hence its computation is not simple. It is our choice of $\Psi(t)$ that makes this term zero, and hence makes it possible to avoid this computation.

We now turn to the analysis of $\widehat{T}_{n,n'}[f]$.

Let us define

$$v(\theta) = \int_0^{2\pi} F(\theta, \phi)\mathrm{d}\phi, \qquad \widehat{v}(t) = \int_0^1 \widehat{F}(t, \phi)\mathrm{d}\phi.$$

Thus,

$$\widehat{v}(t) = v(\Psi(t), \phi)\,\Psi'(t), \qquad I[f] = \int_0^{\pi} v(\theta)\mathrm{d}\theta = \int_0^1 \widehat{v}(t)\mathrm{d}t.$$

Note that the integral $\int_0^1 \widehat{v}(t)\mathrm{d}t$ is obtained from $\int_0^{\pi} v(\theta)\mathrm{d}\theta$ by transforming the variable θ via $\theta = \Psi(t)$. Let us denote by $\widetilde{T}_n[f]$ the trapezoidal rule approximation to the one-dimensional integral $\int_0^1 \widehat{v}(t)\mathrm{d}t$. Thus, because $\widehat{F}(0, \phi) = \widehat{F}(1, \phi) = 0$,

$$\widetilde{T}_n[f] = h \sum_{j=1}^{n-1} \widehat{v}(jh). \tag{6.6}$$

In [13, Section 3] (see also [15, Section 2]), we proved that, provided $n' \sim \alpha n^{\beta}$ as $n \to \infty$ for some fixed positive α and β, there holds

$$\widehat{T}_{n,n'}[f] - I[f] = \big(\widetilde{T}_n[f] - I[f]\big) + O(h^{\nu}) \quad \text{as } n \to \infty, \text{ for every } \nu > 0. \tag{6.7}$$

It is clear from this that, despite being different from each other, $\widehat{T}_{n,n'}[f] - I[f]$ and $\widetilde{T}_n[f] - I[f]$ have the same asymptotic expansions as $h \to 0$. Thus, it is enough to analyze $\widetilde{T}_n[f] - I[f]$. For this, it is sufficient to know the asymptotic expansions of $v(\theta)$ as $\theta \to 0$ and $\theta \to \pi$, as we have seen in the preceding sections. These asymptotic expansions of $v(\theta)$ have already been obtained in [15, Sections 3 and 4] and are summarized in [15, Theorem 4.2], which we reproduce next.

Theorem 6.1. (i) *When the singularity of $f(Q)$ is mapped to the north pole of the unit sphere,*

$$v(\theta) \sim \sum_{i=0}^{\infty} \mu_i^{(+,0)} \theta^{2i} \quad \text{as } \theta \to 0, \qquad v(\theta) \sim \sum_{i=0}^{\infty} \mu_i^{(+,\pi)} (\pi - \theta)^{2i+1} \quad \text{as } \theta \to \pi. \tag{6.8}$$

(ii) *When the singularity of $f(Q)$ is mapped to the south pole of the unit sphere,*

$$v(\theta) \sim \sum_{i=0}^{\infty} \mu_i^{(-,0)} \theta^{2i+1} \quad \text{as } \theta \to 0, \qquad v(\theta) \sim \sum_{i=0}^{\infty} \mu_i^{(-,\pi)} (\pi - \theta)^{2i} \quad \text{as } \theta \to \pi. \tag{6.9}$$

The following theorem, whose proof is precisely as those of Theorem 4.2 in [12] and Theorem 6.2 in [15], presents the optimal result that can be obtained from $\widehat{T}_{n,n'}[f]$. It can be proved by first applying part (ii) of Theorem 4.2 to the integral $\int_0^{\pi} v(\theta)\mathrm{d}\theta = \int_0^1 \widehat{v}(t)\mathrm{d}t$ in view of Theorem 6.1, and by invoking (6.7) next.

Theorem 6.2. *Let $\Psi(t)$ be as in (6.3), and let $n' \sim \alpha n^{\beta}$ as $n \to \infty$ for some fixed positive α and β (for example, $n' = n$). Then*

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

In the case where $2m$ is an odd integer, the complete asymptotic expansion of $\widehat{T}_{n,n'}[f]$ is of the form

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

Note that there is no contribution to the asymptotic expansion of the error $\widehat{T}_{n,n'}[f] - I[f]$ from the pole to which the point singularity is mapped.

7. Example: Numerical integration over surfaces of ellipsoids

Let S be the surface of the ellipsoid whose equation is $(\xi/a)^2+(\eta/b)^2+(\zeta/c)^2 = 1$, and let $f(Q) = g(Q)/|Q-P|$, with $g(Q) = g(\xi,\eta,\zeta) = \exp[0.1(\xi + 2\eta + 3\zeta)]$. We take $(a,b,c) = (1, 2, 3)$ and $P = (\xi_0, \eta_0, \zeta_0) = (1/2,\ 1,\ 3/\sqrt{2}) \in S$, and consider the computation of the integral

$$I[f] = \iint_S f(Q)\mathrm{d}A_S = 38.2549189698039\cdots.$$

This is one of the numerical examples treated in Atkinson [2] and in Sidi [15].

Letting

$$U = \left\{(x,y,z):\ x^2+y^2+z^2 = 1\right\},$$

we take the mapping of U to S to be

$$(\xi,\eta,\zeta) = (ax, by, cz),$$

by which P is the mapping of

$$(x_0, y_0, z_0) = (\xi_0/a, \eta_0/b, \zeta_0/c) = (1/2, 1/2, 1/\sqrt{2}) \in U.$$

This point is mapped to the south pole via the (orthogonal) Householder matrix H,

$$H = I - 2pp^{\mathrm{T}}, \qquad p = \frac{1}{\sqrt{2+\sqrt{2}}}\begin{bmatrix} 1/2 \\ 1/2 \\ 1/\sqrt{2}+1 \end{bmatrix};$$

that is,

$$\begin{bmatrix} x_0 \\ y_0 \\ z_0 \end{bmatrix} = H \begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} x \\ y \\ z \end{bmatrix} = H \begin{bmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{bmatrix}.$$

The function $F(\theta,\phi)$ is given as in

$$F(\theta,\phi) = f(\xi,\eta,\zeta)R(x,y,z)\sin\theta,$$

where

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

The numerical results in Tables 5 and 6, which were computed with $\Psi(t) = \pi\psi_{m,2}(t)$, in quadruple-precision arithmetic, illustrate the conclusions of Theorem 6.2 very clearly. Table 5 gives the relative errors in the $\widehat{T}_n[f] \equiv \widehat{T}_{n,n}[f]$, $n = 2^k$, $k = 1, 2, \ldots, 9$, for various values of m. Table 6 presents the numbers

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

for the same values of m and for $k = 1, 2, \ldots, 8$. It is seen that, with increasing k, the $\rho_{m,k}$ in Table 6 are tending to $4m+4$ when $2m$ is an odd integer, while they are tending to $2m+2$ for other values of m, completely in accordance

Table 5
Relative errors in the rules $\widehat{T}_n[f] = \widehat{T}_{n,n}[f]$ for the integral of Section 7, obtained with $n = 2^k$, $k = 1(1)9$, and with the $\sin^{m,2}$-transformation

n	$m = 0.5$	$m = 1$	$m = 1.5$	$m = 2$	$m = 2.5$	$m = 3$	$m = 3.5$	$m = 4$	$m = 4.5$	$m = 5$
2	2.06D+01	3.28D+01	3.09D+01	1.84D+01	3.72D+00	8.63D+00	1.78D+01	2.41D+01	2.85D+01	3.14D+01
4	2.42D−01	2.65D+00	3.13D+00	1.62D+00	1.32D−01	1.23D+00	1.57D+00	1.29D+00	5.83D−01	4.16D−01
8	2.83D−02	4.66D−03	2.27D−02	8.98D−02	3.72D−02	1.01D−01	1.79D−01	1.14D−01	6.88D−02	2.91D−01
16	5.78D−04	4.97D−04	5.99D−04	5.01D−04	6.57D−04	7.08D−04	2.82D−04	2.17D−04	7.36D−04	1.24D−03
32	2.19D−08	4.26D−06	3.12D−08	2.09D−08	2.69D−08	4.61D−08	2.84D−09	7.33D−08	8.08D−08	2.47D−07
64	8.24D−10	2.64D−07	1.77D−15	1.46D−10	1.42D−16	1.50D−13	2.02D−15	5.73D−15	2.50D−14	2.01D−14
128	1.29D−11	1.65D−08	1.63D−18	2.27D−12	8.88D−25	5.85D−16	1.56D−30	2.37D−19	2.44D−27	1.37D−22
256	2.01D−13	1.03D−09	1.59D−21	3.55D−14	5.40D−29	2.28D−18	6.78D−32	2.31D−22	6.16D−32	3.35D−26
512	3.14D−15	6.44D−11	1.56D−24	5.55D−16	2.47D−32	8.92D−21	4.31D−32	2.25D−25	7.40D−32	8.21D−30

Table 6
The numbers $\rho_{m,k} = \frac{1}{\log 2} \cdot \log\left(\frac{|\widehat{T}_{2^k}[f]-I[f]|}{|\widehat{T}_{2^{k+1}}[f]-I[f]|}\right)$, with m, $f(x)$, and $\widehat{T}_n[f]$ as in Table 5, for $k = 1(1)8$

k	$m = 0.5$	$m = 1$	$m = 1.5$	$m = 2$	$m = 2.5$	$m = 3$	$m = 3.5$	$m = 4$	$m = 4.5$	$m = 5$
1	6.410	3.626	3.302	3.500	4.817	2.807	3.502	4.224	5.609	6.238
2	3.095	9.153	7.109	4.176	1.826	3.608	3.132	3.497	3.084	0.513
3	5.613	3.230	5.242	7.487	5.824	7.157	9.307	9.043	6.546	7.872
4	14.689	6.864	14.229	14.550	14.577	13.907	16.600	11.531	13.153	12.301
5	4.732	4.013	24.075	7.162	27.500	18.233	20.423	23.607	21.622	23.549
6	6.002	4.001	10.078	6.001	27.247	7.999	50.202	14.565	43.225	27.125
7	6.000	4.000	10.002	6.000	14.005	8.001	4.524	10.001	15.271	12.002
8	6.000	4.000	10.000	6.000	11.098	8.000	0.652	10.000	−0.263	11.994
∞	6	4	10	6	14	8	18	10	22	12

with Theorem 6.2. Note that the results with $2m$ an odd integer in Tables 5 and 6 are very similar to the corresponding results in [15, Tables 3 and 4] that were obtained with a transformation different from the $\sin^{m,2}$-transformation.

From the analysis given in [15, Section 6, Lemma 6.1], it becomes clear that the variable transformation used there, namely, $\Psi(t) = \Psi_{2,S}(t) = 2\pi\psi(\frac{1}{2}\varpi(t))$, with $\psi \in \mathcal{S}_m$ and $\varpi \in \mathcal{S}_q$, q being an even integer, is in the class $\mathcal{S}_{M,q}$, where $M = (q+1)(m+1) - 1$.

8. Comparison with some recent transformations

In a recent paper by the author [16], a new class of symmetric and nonsymmetric variable transformations denoted as $\mathcal{T}_{r,s}$ was designed, and it was shown there how some members of this class can be constructed easily. Now, $\phi \in \mathcal{T}_{r,s}$, $r, s > 0$, if

1. $\phi \in C[0,1]$ and $\phi \in C^\infty(0,1)$; $\phi(0) = 0$, $\phi(1) = 1$, and $\phi'(t) > 0$ on $(0,1)$.
2. $\phi(t)$ has the following asymptotic expansions as $t \to 0+$ and $t \to 1-$:

$$\begin{aligned} &\phi(t) \sim \sum_{i=0}^{\lfloor r/2 \rfloor} \alpha_i t^{r+2i} + \sum_{i=0}^{\infty} \tilde{\alpha}_i t^{\sigma_i} \quad \text{as } t \to 0+; \quad \alpha_0 > 0, \\ &\phi(t) \sim 1 - \sum_{i=0}^{\lfloor s/2 \rfloor} \beta_i (1-t)^{s+2i} - \sum_{i=0}^{\infty} \tilde{\beta}_i (1-t)^{\rho_i} \quad \text{as } t \to 1-; \quad \beta_0 > 0, \end{aligned} \tag{8.1}$$

where

$$\begin{aligned} &2r = \sigma_0 < \sigma_1 < \cdots; \quad \lim_{i\to\infty} \sigma_i = \infty, \\ &2s = \rho_0 < \rho_1 < \cdots; \quad \lim_{i\to\infty} \rho_i = \infty. \end{aligned} \tag{8.2}$$

3. For each positive integer k, $\phi^{(k)}(t)$ has asymptotic expansions as $t \to 0+$ and $t \to 1-$ that are obtained by differentiating those of $\phi(t)$ term by term k times.

Possibly the simplest member of $\mathcal{T}_{r,s}$ is $\phi(t) = (\sin \frac{\pi}{2}t)^r / [(\sin \frac{\pi}{2}t)^r + (\cos \frac{\pi}{2}t)^s]$, and this was given in [16].

Comparing (8.1) with (2.2), we notice that the class $\mathcal{T}_{p+1,q+1}$ is analogous to $\mathcal{S}_{p,q}$, but the two are different. When p and q are chosen optimally, transformations in $\mathcal{T}_{p+1,q+1}$ are in some cases as good as those in $\mathcal{S}_{p,q}$. There are some important cases for which transformations in $\mathcal{S}_{p,q}$ are superior. This is borne out by a comparison of parts (ii) (concerning *optimal* choices of p, q and r, s) in Theorem 4.2 of the present work and Theorem 3.2 in [16]. We have the following:

Theorem 8.1. *Assume all the conditions of Theorem 4.2, with the notation therein. Given that γ_0 and δ_0 are both real, choose $p = (2k - \gamma_0)/(\gamma_0 + 1)$ and $q = (2l - \delta_0)/(\delta_0 + 1)$, where k and l are positive integers. Let $\widehat{Q}_n[f]$ be the trapezoidal rule applied to the integrand $f_1(t) \equiv f(\psi(t))\psi'(t)$ with $\psi \in \mathcal{S}_{p,q}$, or to the integrand $f_2(t) \equiv f(\phi(t))\phi'(t)$ with $\phi \in \mathcal{T}_{p+1,q+1}$. Then*

$$\widehat{Q}_n[f] - I[f] = O\left(h^{\omega_i}\right) \quad \text{as } h \to 0,$$

where

$$\omega_1 = \min\{(\Re\gamma_1 + 1)(p+1), (\Re\delta_1 + 1)(q+1)\} \quad \text{for } f_1(t),$$

and

$$\omega_2 = \min\{(\gamma_0 + 2)(p+1), (\Re\gamma_1 + 1)(p+1), (\delta_0 + 2)(q+1), (\Re\delta_1 + 1)(q+1)\} \quad \text{for } f_2(t).$$

Clearly, $\omega_1 \geq \omega_2$ always, which means that class $\mathcal{S}_{p,q}$ transformations perform always at least as well as class $\mathcal{T}_{p+1,q+1}$ transformations. Their performances are the same, that is, $\omega_1 = \omega_2$, only when $\gamma_0 + 2 = \Re\gamma_1 + 1$ and $\delta_0 + 2 = \Re\delta_1 + 1$; otherwise, $\omega_1 > \omega_2$.

Let us consider the case $f \in \mathbb{C}^\infty[0, 1]$. (i) If $f(0) \neq 0$, $f(1) \neq 0$ and $f'(0) \neq 0$, $f'(1) \neq 0$, we have $\gamma_0 = \delta_0 = 0$ and $\gamma_1 = \delta_1 = 1$. Then, with (optimal) $p = q = 2k$, $k = 1, 2, \ldots$, we have $\omega_1 = \omega_2 = 2(p+1)$. (ii) If $f(0) \neq 0$, $f(1) \neq 0$ but $f'(0) = f'(1) = 0$, then we have $\gamma_0 = \delta_0 = 0$, $\gamma_1 = \delta_1 = 2$, and γ_2 and δ_2 are at least 3. Then with (optimal) $p = q = 2k$, $k = 1, 2, \ldots$, we have $\omega_2 = 2(p+1)$. Because $2(p+1) + p$ is an even integer, there is no contribution to the error involving $\gamma_1 = \delta_1$, and now $\omega_1 \geq c(p+1)$, where $c = \min\{(\gamma_2 + 1), (\delta_2 + 1)\}$, so that $\omega_1 \geq 4(p+1)$. Hence $\omega_1 \geq 2\omega_2$ in this case.

As another example, let us look at the product trapezoidal rule for the two-dimensional integrals that we discussed in Section 6. If we replace the class $\mathcal{S}_{m,2}$ (class $\mathcal{S}_{2,m}$) transformations in (6.3) by class $\mathcal{T}_{m+1,q+1}$ (class $\mathcal{T}_{q+1,m+1}$) transformations with (optimal) $m = (2k-1)/2$ and $q = 2l$, where k and l are positive integers, then $\omega_2 = \min\{3(m+1), 2(q+1)\} \leq 3(m+1)$, as opposed to $\omega_1 = 4(m+1)$ that we obtained in Theorem 6.2. Thus, $\omega_1 \geq \frac{4}{3}\omega_2$ for the integrals being discussed.

A further class of nonsymmetric variable transformations based on [6, Section 2] was considered in [16, Section 5] and denoted as $\widetilde{\mathcal{T}}_{r,s}$. Functions in this class differ from those in $\mathcal{T}_{r,s}$ in that their asymptotic expansions as $t \to 0+$ and $t \to 1-$ are of the form

$$\begin{aligned} \phi(t) &\sim \sum_{i=0}^{2\lfloor r/2 \rfloor} \alpha_i t^{r+i} + O\left(t^{2r}\right) \quad \text{as } t \to 0+; \quad \alpha_0 > 0, \\ \phi(t) &\sim 1 - \sum_{i=0}^{2\lfloor s/2 \rfloor} \beta_i (1-t)^{s+i} + O\left((1-t)^{2s}\right) \quad \text{as } t \to 1-; \quad \beta_0 > 0. \end{aligned} \tag{8.3}$$

Transformations in $\widetilde{\mathcal{T}}_{r,s}$ are compared with those in $\mathcal{T}_{r,s}$ in Theorem 5.1 of [16]. It follows from this theorem that, when used with optimal r and s, the latter perform better on regular integrands and on integrands with algebraic endpoint singularities.

Thus, we conclude that, when applied with optimal p and q, transformations in $\mathcal{S}_{p,q}$ perform better than those in $\mathcal{T}_{p+1,q+1}$, which perform better than those in $\widetilde{\mathcal{T}}_{p+1,q+1}$.

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