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A Novel Class of Symmetric and Nonsymmetric Periodizing Variable Transformations for Numerical Integration

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Variable transformations for numerical integration have been used for improving the accuracy of the trapezoidal rule. Specifically, one first transforms the integral $I[f]=\int_0^1 f(x)\,dx$ via a variable transformation $x=\phi(t)$ that maps [0, 1] to itself, and then approximates the resulting transformed integral $I[f]=\int_0^1 f\big(\phi(t)\big)\phi'(t)\,dt$ by the trapezoidal rule. In this work, we propose a new class of symmetric and nonsymmetric variable transformations which we denote $\mathcal{T}_{r,s}$, where r and s are positive scalars assigned by the user. A simple representative of this class is $\phi(t)=(\sin\frac{\pi}{2}t)^r/[(\sin\frac{\pi}{2}t)^r+(\cos\frac{\pi}{2}t)^s]$. We show that, in case $f\in C^\infty[0,1]$, or $f\in C^\infty(0,1)$ but has algebraic (endpoint) singularities at $x=0$ and/or $x=1$, the trapezoidal rule on the transformed integral produces exceptionally high accuracies for special values of r and s. In particular, when $f\in C^\infty[0,1]$ and we employ $\phi\in\mathcal{T}_{r,r}$, the error in the approximation is (i) $O(h^r)$ for arbitrary r and (ii) $O(h^{2r})$ if r is a positive odd integer at least 3, h being the integration step. We illustrate the use of these transformations and the accompanying theory with numerical examples.

KEY WORDS: Numerical integration; variable transformations, $\sin^m$-transformation, Euler–Maclaurin expansions; asymptotic expansions; trapezoidal rule.

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1. INTRODUCTION AND BACKGROUND

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

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

where $f\in C^\infty(0,1)$ but is not necessarily continuous or differentiable at $x=0$ and/or $x=1$, and may even have different types of singularities at the endpoints. 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

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

and $I[f]$ can be approximated by applying the trapezoidal rule to $\int_0^1 \widehat{f}(t)dt$, namely, by

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

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 the function $\widehat{f}(t)$ is such that $\widehat{f}^{(i)}(0)=\widehat{f}^{(i)}(1)=0, i=1,2,\dots,q$, for some q. Thus, from the Euler–Maclaurin expansion of $\widehat{Q}_n[f]$ (see, e.g., Davis and Rabinowitz [5] or Stoer and Bulirsch [19] or Atkinson [2] or Sidi [10, Appendix D]), it follows that $\widehat{Q}_n[f]-I[f]=o(n^{-q})$ as $n\to\infty$, which means that $\widehat{Q}_n[f]$ approximates $I[f]$ with surprisingly high accuracy even for moderate n. In such a case, we also have $\widehat{f}(0)=\widehat{f}(1)=0$, and $\widehat{Q}_n[f]$ assumes the simpler form

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

Variable transformations in numerical integration, especially in the presence of integrands with endpoint singularities, 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, as we have already mentioned. They have also been used by Verlinden et al. [20], in conjunction with extrapolation methods, to improve the performance of the product trapezoidal rule in multiple integration. Recently, they have been used to improve the performance of the Gauss–Legendre quadrature; see, for example, Monegato and Scuderi [7] and Johnston [6]. 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; see, for example, Sloan and Joe [18] and Robinson and Hill [8]. (Lattice rules are extensions of the trapezoidal rule to many dimensions.) They have also been used in conjunction with the product trapezoidal rule in computing integrals over surfaces of spheres in three dimensions and, more generally, on surfaces of bounded sets in $\mathbb{R}^3$; see Atkinson [3], Atkinson and Sommariva [4], and Sidi [12–14, 17].

Normally, we also demand that $\psi(t)$ be *symmetric*, in the sense that $\psi(1-t) = 1 - \psi(t)$, which forces on $\psi'(t)$ the symmetry property $\psi'(1-t) = \psi'(t)$. Most variable transformations are indeed symmetric in this sense. However, as discussed by Monegato and Scuderi [7], by employing *nonsymmetric* variable transformations, we can cope with integrands having singularities of *different* strengths at the endpoints more efficiently. Actually, these authors show exactly how to modify the known symmetric transformations in simple ways to obtain nonsymmetric ones.

Following Monegato and Scuderi [7] and Sidi [15], in [16], the author developed a class of nonsymmetric variable transformations, denoted $\mathcal{S}_{p,q}$, that is defined as follows:

Definition 1.1. 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 $t \to 1-$:

$$\begin{aligned} \psi'(t) &\sim \sum_{i=0}^{\infty} \epsilon_i t^{p+2i} \quad \text{as} \quad t \to 0+, \\ \psi'(t) &\sim \sum_{i=0}^{\infty} \delta_i (1-t)^{q+2i} \quad \text{as} \quad t \to 1-, \end{aligned} \tag{1.5}$$

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

$$\begin{aligned} \psi(t) &\sim \sum_{i=0}^{\infty} \epsilon_i \frac{t^{p+2i+1}}{p+2i+1} \quad \text{as} \quad t \to 0+, \\ \psi(t) &\sim 1 - \sum_{i=0}^{\infty} \delta_i \frac{(1-t)^{q+2i+1}}{q+2i+1} \quad \text{as} \quad t \to 1-. \end{aligned} \tag{1.6}$$

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.

A representative of this class is the $\sin^{p,q}$-transformation defined as in

$$\psi_{p,q}(t) = \frac{\Theta_{p,q}(t)}{\Theta_{p,q}(1)}; \quad \Theta_{p,q}(t) = \int_0^t \left(\sin \tfrac{\pi}{2} u\right)^p \left(\cos \tfrac{\pi}{2} u\right)^q du, \quad p, q > 0. \tag{1.7}$$

This transformation is the nonsymmetric generalization of the $\sin^m$-transformation of the author (proposed originally with integer m in [9], and extended to arbitrary values of m recently in [15]) and was proposed with *integer* p and q in [7]. With integer p and q, it can be computed recursively, as shown in [7]. In [16], the $\sin^{p,q}$-transformation was extended to *arbitrary* and not necessarily integer p and q to enhance their effectiveness. When either p or q or both are not integers, $\psi_{p,q}(t)$ cannot be computed by recursions because initial values are not readily available. In such cases, $\psi_{p,q}(t)$ can be computed by summing a quickly converging infinite series representation, as shown in [16]. Also, when $p = q = m$, the $\sin^{p,q}$-transformation becomes the (symmetric) $\sin^m$-transformation. Both when $p = q$ and $p \neq q$, the $\sin^{p,q}$-transformation can be expressed in terms of the hypergeometric function $F(a, b; c; z) = {}_2F_1(a, b; c; z)$, among others, in the form

$$\psi_{p,q}(t) = \frac{F\left(\frac{1}{2} - \frac{1}{2}q, \frac{1}{2}p + \frac{1}{2}; \frac{1}{2}p + \frac{3}{2}; S^2\right)}{F\left(\frac{1}{2} - \frac{1}{2}q, \frac{1}{2}p + \frac{1}{2}; \frac{1}{2}p + \frac{3}{2}; 1\right)} S^{p+1}, \quad S = \sin \frac{\pi t}{2}. \tag{1.8}$$

A complete analysis of the trapezoidal rule approximations $\widehat{Q}_n[f]$ as given in (1.4), with $\psi(t) \in \mathcal{S}_{p,q}$ there, was also provided in [16]. In order to motivate the developments of the present work, we need to recall Theorem 4.2 and Corollary 4.3 in [16], which are the main results of [16]. These are given as Theorem 1.2 and Corollary 1.3 below:

Theorem 1.2. Let $f \in C^\infty(0, 1)$, and assume that $f(x)$ has the asymptotic expansions

$$f(x) \sim \sum_{i=0}^{\infty} c_i x^{\gamma_i} \quad \text{as } x \to 0+; \quad f(x) \sim \sum_{i=0}^{\infty} d_i (1 - x)^{\delta_i} \quad \text{as } x \to 1-.$$

Here γ_i and δ_i are distinct complex numbers that satisfy

$$-1 < \Re\gamma_0 \leqslant \Re\gamma_1 \leqslant \Re\gamma_2 \leqslant \cdots; \lim_{i\to\infty} \Re\gamma_i = +\infty,$$
$$-1 < \Re\delta_0 \leqslant \Re\delta_1 \leqslant \Re\delta_2 \leqslant \cdots; \lim_{i\to\infty} \Re\delta_i = +\infty.$$

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 $I[f] = \int_0^1 f(x)\,dx$, 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 $\widehat{Q}_n[f] = \sum_{i=1}^{n-1} f\big(\psi(ih)\big)\psi'(ih)$, where $h = 1/n$, $n = 1, 2, \ldots$. Then the following hold:

(i) In the worst case,

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

(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

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

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 $\gamma_i = \mu + i$ and $\delta_i = \nu + i$, $i = 0, 1, \ldots$. 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.

Corollary 1.3. In case $f(x) = x^{\mu}(1 - x)^{\nu}g(x)$, $g(x)$ being infinitely differentiable on [0, 1], the following hold:

(i) In the worst case,

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

(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

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

at worst.

Remark. Note that the results in parts (ii) of Theorem 1.2 and Corollary 1.3 are the best that can be obtained and are made possible by our definition of the class $\mathcal{S}_{p,q}$ transformations, where we have excluded the powers t^{p+2i+1} and $(1-t)^{q+2i+1}$, $i=0,1,\dots,$ from the asymptotic expansions of $\psi'(t)$ as $t\to 0+$ and $t\to 1-$.

Now, in [15], we introduced the concept of *quality* of $\widehat{Q}_n[f]$ in a way that is relevant to symmetric variable transformations. Here we modify this concept to make it relevant to nonsymmetric transformations in $\mathcal{S}_{p,q}$ as follows: If $\psi'(t)\sim \alpha t^p$ as $t\to 0+$ and $\psi'(t)\sim \beta(1-t)^q$ 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/w, where $w=\max\{p+1,q+1\}$. 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 p and 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 $\mathcal{S}_{p,q}$ with special (not necessarily integer) values of p and q.

In view of what we have described so far, we now address ourselves to the following question: Are there variable transformations $\psi(t)$ that are not in $\mathcal{S}_{p,q}$ with the properties that (i) they satisfy $\psi(t)\sim\epsilon t^{p+1}$ as $t\to 0+$ and $\psi(t)\sim 1-\delta(1-t)^{q+1}$ as $t\to 1-$ just as those in $\mathcal{S}_{p,q}$ do, (ii) are easy to compute, and (iii) Theorem 1.2 and Corollary 1.3 remain unchanged in their presence?

In this work, we propose a novel class of variable transformations, which we denote $\mathcal{T}_{r,s}$, that have these properties in general. The members of $\mathcal{T}_{r,s}$ are analogous to those of $\mathcal{S}_{r-1,s-1}$, and although they differ from the latter substantially, they have similar properties. In particular, there are analogues of Theorem 1.2 and Corollary 1.3 that pertain to members of $\mathcal{T}_{r,s}$ and that say that, in general, whatever can be done with variable transformations in $\mathcal{S}_{r-1,s-1}$ can be done also with those in $\mathcal{T}_{r,s}$. In addition, we have been able to produce transformations in $\mathcal{T}_{r,s}$ that are easier to compute than those in the classes $\mathcal{S}_{p,q}$.

In the next section, we define the class $\mathcal{T}_{r,s}$ and show how transformations in this class can be determined easily. We provide a remarkably simple and easily computable representative of it, which we denote the $T^{r,s}$-transformation. When $r=s$, this transformation, denoted the T^r-transformation for short, is symmetric. In Section 3, we provide the convergence theory of the trapezoidal rule approximations $\widehat{Q}_n[f]$ obtained using members of $\mathcal{T}_{r,s}$. We also show how the performance of our approach can be improved substantially by subtracting from the integrand a simple function with known integral. In Section 4, we provide numerical examples that illustrate the theory. We use the $T^{r,s}$-transformation in these examples. Finally, in Section 5, we discuss an already existing modification of the class proposed here, and show that it is inferior to the class $\mathcal{T}_{r,s}$.

To distinguish the variable transformations in $\mathcal{T}_{r,s}$ from those in $\mathcal{S}_{p,q}$, in the sequel, we will denote them by $\phi(t)$ instead of $\psi(t)$.

2. THE CLASS $\mathcal{T}_{r,s}$

2.1. Definition of the Class $\mathcal{T}_{r,s}$

Definition 2.1. A function $\phi(t)$ is in the class $\mathcal{T}_{r,s}$, with $r, s > 0$ but arbitrary, if it has the following properties:

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 $t \to 1-$:

$$\phi\ (t) \sim \sum_{i=0}^{\lfloor r/2 \rfloor} \alpha_i t^{r+2i} + \sum_{i=0}^{\infty} \tilde{\alpha}_i t^{\sigma_i} \quad \text{as } t \to 0+; \quad \alpha_0 > 0,$$
$$\phi\ (t) \sim 1 - \sum_{i=0}^{\lfloor s/2 \rfloor} \beta_i (1-t)^{s+2i} - \sum_{i=0}^{\infty} \tilde{\beta}_i (1-t)^{\rho_i} \quad \text{as } t \to 1-; \quad \beta_0 > 0, \tag{2.1}$$

where

$$2r = \sigma_0 < \sigma_1 < \cdots; \quad \lim_{i\to\infty} \sigma_i = \infty,$$
$$2s = \rho_0 < \rho_1 < \cdots; \quad \lim_{i\to\infty} \rho_i = \infty. \tag{2.2}$$

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. In particular, $\phi'(t)$ has the following asymptotic expansions as $t \to 0+$ and $t \to 1-$:

$$\phi'\ (t) \sim \sum_{i=0}^{\lfloor r/2 \rfloor} (r+2i)\alpha_i t^{r+2i-1} + \sum_{i=0}^{\infty} \sigma_i \tilde{\alpha}_i t^{\sigma_i - 1} \quad \text{as } t \to 0+,$$
$$\phi'\ (t) \sim \sum_{i=0}^{\lfloor s/2 \rfloor} (s+2i)\beta_i (1-t)^{s+2i-1} + \sum_{i=0}^{\infty} \rho_i \tilde{\beta}_i (1-t)^{\rho_i - 1} \quad \text{as } t \to 1-. \tag{2.3}$$

Remarks. 1. From Definition 2.1, it is clear that $\phi \in \mathcal{T}_{r,s}$ satisfies

$$\begin{aligned} \phi(t) &= \sum_{i=0}^{\lfloor r/2 \rfloor} \alpha_i t^{r+2i} + O\left(t^{2r}\right) \quad \text{as } t \to 0+, \\ \phi(t) &= 1 - \sum_{i=0}^{\lfloor s/2 \rfloor} \beta_i (1-t)^{s+2i} + O\left((1-t)^{2s}\right) \quad \text{as } t \to 1-, \end{aligned} \tag{2.4}$$

and

$$\begin{aligned} \phi'(t) &= \sum_{i=0}^{\lfloor r/2 \rfloor} (r+2i)\alpha_i t^{r+2i-1} + O\left(t^{2r-1}\right) \quad \text{as } t \to 0+, \\ \phi'(t) &= \sum_{i=0}^{\lfloor s/2 \rfloor} (s+2i)\beta_i (1-t)^{s+2i-1} + O\left((1-t)^{2s-1}\right) \quad \text{as } t \to 1-. \end{aligned} \tag{2.5}$$

2. As we will see in Section 3, what makes class $\mathcal{T}_{r,s}$ transformations effective is the fact that we have excluded the powers t^{r+2i+1}, $i = 0, 1, \ldots, \lfloor r/2 \rfloor - 1$, and $(1-t)^{s+2i+1}$, $i = 0, 1, \ldots, \lfloor s/2 \rfloor - 1$, from the asymptotic expansions of $\phi(t)$ as $t \to 0+$ and $t \to 1-$, respectively.

To keep the developments below and the notation simple, we give two definitions.

Definition 2.2. We denote generically by $R_\mu(t)$ any function $g(t)$ that has an asymptotic expansion of the form

$$g(t) \sim \sum_{i=0}^{\infty} r_i t^{\mu+2i} \quad \text{as } t \to 0+.$$

Remark. Note that, in Definition 2.2, we do not require $r_0 \neq 0$, because such a requirement is not needed in the sequel.

By Definition 2.2, we have

$$R_\mu(t) + R_{\mu+2j}(t) = R_\mu(t), \quad j = 0, 1, 2, \ldots, \tag{2.6}$$

hence

$$\sum_{j=0}^{\infty} R_{\mu+2j}(t) = R_\mu(t). \tag{2.7}$$

In addition,

$$[R_\mu(t)]^\alpha = R_{\alpha\mu}(t) \quad \text{and} \quad R_\mu(t)R_\nu(t) = R_{\mu+\nu}(t). \tag{2.8}$$

In case

$$\Re\mu_1 < \Re\mu_2 < \cdots; \quad \lim_{k\to\infty} \Re\mu_k = +\infty, \tag{2.9}$$

and

$$R_{\mu_k}(t) \sim r_{k,0} t^{\mu_k} \quad \text{as } t \to 0+; \quad r_{k,0} \neq 0, \quad k = 1, 2, \dots, \tag{2.10}$$

there holds

$$\lim_{t\to 0+} \frac{R_{\mu_{k+1}}(t)}{R_{\mu_k}(t)} = 0, \quad k = 1, 2, \dots, \tag{2.11}$$

that is, the sequence $\{R_{\mu_k}(t)\}_{k=1}^{\infty}$ is an asymptotic scale as $t \to 0+$.

If $R_\mu(t)$ can be differentiated term by term, we have

$$\frac{d}{dt} R_\mu(t) = R_{\mu-1}(t). \tag{2.12}$$

If $R_\mu(t)$ can be integrated term by term, we have

$$\int_0^t R_\mu(u)\, du = R_{\mu+1}(t). \tag{2.13}$$

We will make free use of all this in the sequel.

Definition 2.3. We say that a function $g(t)$ belongs to the set $\mathcal{K}_\mu$, $\mu > 0$, if

$$g(0) = 0, \quad g(1) = 1; \quad g \in C^\infty(0, 1), \quad g'(t) > 0 \quad \text{for } t \in (0, 1),$$

and if $g(t)$ has asymptotic expansions as $t \to 0+$ and as $t \to 1-$ given as

$$g(t) \sim \sum_{i=0}^{\infty} g_i^{(0)}\, t^{\mu+2i} \quad \text{as } t \to 0+; \quad g_0^{(0)} > 0,$$
$$g(t) \sim \sum_{i=0}^{\infty} g_i^{(1)}\, (1-t)^{2i} \quad \text{as } t \to 1-; \quad g_0^{(1)} = 1,$$

and if, for each $k = 1, 2, \dots,$ the kth derivative of $g(t)$ has asymptotic expansions as $t \to 0+$ and $t \to 1-$ that are obtained by differentiating those of $g(t)$ term by term k times.

Remark. Note that the function $g(t)=t^p$, $p>0$, even though it shares some of the properties of functions in $\mathcal{K}_p$, does not belong to the set $\mathcal{K}_p$.

The following conclusions can easily be drawn from Definition 2.3:

$$g\in\mathcal{K}_\mu \;\Rightarrow\; g(t)=\begin{cases} R_\mu(t) & (\text{for } t\to 0+) \\ R_0(1-t) & (\text{for } t\to 1-) \end{cases}.$$

$$g\in\mathcal{K}_\mu \;\Rightarrow\; u(t)=[g(t)]^\nu\in\mathcal{K}_{\mu\nu} \quad \text{if } \nu>0.$$

$$g_1\in\mathcal{K}_\mu,\;\; g_2\in\mathcal{K}_\nu \;\Rightarrow\; u(t)=g_1(t)g_2(t)\in\mathcal{K}_{\mu+\nu}.$$

We will make use of these properties of functions in the sets $\mathcal{K}_\mu$ shortly.

2.2. Construction of Functions in $\mathcal{T}_{r,s}$

We now propose one simple way of constructing some functions in $\mathcal{T}_{r,s}$: Let $u(t)$ and $v(t)$ be such that

$$u(0)=0,\quad u(1)=1;\quad u\in C^\infty(0,1),\quad u'(t)>0 \quad \text{for } t\in(0,1),$$
$$v(0)=0,\quad v(1)=1;\quad v\in C^\infty(0,1),\quad v'(t)>0 \quad \text{for } t\in(0,1),$$

Thus, $u(t)>0$ and $v(t)>0$ for $0<t\leqslant 1$ as well. Now set

$$\phi(t)=\frac{u(t)}{u(t)+v(1-t)}.$$

It is easy to see that $u(t)+v(1-t)>0$ for $t\in[0,1]$, and that

$$\phi(0)=0,\quad \phi(1)=1,\quad \phi'(t)=\frac{u'(t)v(1-t)+u(t)v'(1-t)}{[u(t)+v(1-t)]^2}>0 \quad \text{for } 0<t<1.$$

That is, $\phi(t)$ is an increasing function of t for $t\in(0,1)$ and satisfies $0\leqslant\phi(t)\leqslant 1$ for $0\leqslant t\leqslant 1$, and hence is a valid variable transformation.

Note that we also have

$$\phi(t)=1-\frac{v(1-t)}{u(t)+v(1-t)},$$

so that, when $u(t)=v(t)$, there holds $\phi(1-t)=1-\phi(t)$; that is, $\phi(t)$ becomes a symmetric transformation.

We now choose $u(t)$ and $v(t)$ such that $u\in\mathcal{K}_r$ and $v\in\mathcal{K}_s$. Then

$$w_0(t)=\frac{u(t)}{v(1-t)}=R_r(t)=O(t^r)=o(1) \quad \text{as } t\to 0+,$$

hence, for all small $t > 0$, $\phi(t)$ has the convergent expansion

$$\phi(t) = \frac{w_0(t)}{1 + w_0(t)} = \sum_{k=1}^{\infty} (-1)^{k-1} [w_0(t)]^k = \sum_{k=1}^{\infty} R_{kr}(t)$$

that is also a valid asymptotic expansion as $t \to 0+$. Similarly,

$$w_1(t) = \frac{v(1-t)}{u(t)} = R_s(1-t) = O\big((1-t)^s\big) = o(1) \quad \text{as } t \to 1-,$$

hence, for all $t < 1$ but close to 1, $\phi(t)$ has the convergent expansion

$$\phi(t) = 1 - \frac{w_1(t)}{1 + w_1(t)} = 1 - \sum_{k=1}^{\infty} (-1)^{k-1} [w_1(t)]^k = 1 - \sum_{k=1}^{\infty} R_{ks}(1-t)$$

that is also a valid asymptotic expansion as $t \to 1-$. Invoking the properties of the functions $R_\mu(t)$, it is easy to check that $\phi \in \mathcal{T}_{r,s}$ by Definition 2.1. Summarizing, we have

$$u \in \mathcal{K}_r, \ \ v \in \mathcal{K}_s \ \Rightarrow \ \phi(t) = \frac{u(t)}{u(t) + v(1-t)} \in \mathcal{T}_{r,s}.$$

Remark. Recall that the function $g(t) = t^p$, $p > 0$, does not belong to the set $\mathcal{K}_p$. Consequently, the rational transformation $\phi(t) = t^r / [t^r + (1-t)^s]$, defined as explained in the first paragraph of this subsection, and that was first proposed in [7], is not in $\mathcal{T}_{r,s}$.

2.3. Construction of Functions in $\mathcal{K}_\mu$

What remains now is the construction of functions in $\mathcal{K}_\mu$ as inexpensively as possible. Following Definition 2.1, we listed several conclusions pertaining to the class $\mathcal{K}_\mu$. One of these conclusions is that if $g \in \mathcal{K}_\mu$, then $g^\nu \in \mathcal{K}_{\mu\nu}$, which means that, if we know one single function $w \in \mathcal{K}_\sigma$ for some arbitrary σ, we can use it to generate functions $u \in \mathcal{K}_\mu$ for any μ simply via $u(t) = [w(t)]^{\mu/\sigma}$. Such functions are already known to us from previous work: functions in the class $\mathcal{S}_m$, m being an odd integer, are in $\mathcal{K}_{m+1}$, as can be verified by the definition of the class $\mathcal{S}_m$. Recall that if $\psi \in \mathcal{S}_m$, m a positive integer, then

$$\psi \in C^\infty[0,1]; \quad \psi(0) = 0, \quad \psi(1) = 1; \quad \psi'(t) > 0 \text{ on } (0,1),$$

and $\psi(t)$ has asymptotic expansions as $t \to 0+$ and $t \to 1-$ of the forms

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

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

and, 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. (Thus, $\psi \in \mathcal{S}_{m,m}$ as well.)

Choosing two transformations, $\varrho(t) \in \mathcal{S}_k$ and $\varpi(t) \in \mathcal{S}_l$, where k and l are odd positive integers, we set

$$u(t) = [\varrho(t)]^{r/(k+1)} \quad \text{and} \quad v(t) = [\varpi(t)]^{s/(l+1)}.$$

A nice feature of this construction is that we can choose $\varrho(t)$ and $\varpi(t)$ to be simply $\psi_{k-1}(t)$ and $\psi_{l-1}(t)$, namely, the $\sin^{k-1}$ and $\sin^{l-1}$ transformations, respectively, which are readily available at a low computational cost, see [9]. For example,

$$\psi_1(t) = \tfrac{1}{2}(1 - \cos \pi t) = \left(\sin \tfrac{\pi}{2} t\right)^2, \quad \psi_3(t) = \tfrac{1}{16}(8 - 9\cos \pi t + \cos 3\pi t).$$

2.4. The $T^{r,s}$- and T^r-Transformations

Choosing $\varrho(t) = \varpi(t) = \psi_1(t) = (\sin \frac{\pi}{2} t)^2$ in the preceding subsection, we obtain a remarkably simple and readily computable transformation in the class $\mathcal{T}_{r,s}$. We then have $u(t) = (\sin \frac{\pi}{2} t)^r$ and $v(t) = (\sin \frac{\pi}{2} t)^s$, and recalling that $\sin[\frac{\pi}{2}(1-t)] = \cos \frac{\pi}{2} t$, we finally obtain

$$\phi(t) \equiv \phi_{r,s}(t) = \frac{\left(\sin \frac{\pi}{2} t\right)^r}{\left(\sin \frac{\pi}{2} t\right)^r + \left(\cos \frac{\pi}{2} t\right)^s}. \tag{2.14}$$

Therefore,

$$\phi'(t) \equiv \phi_{r,s}'(t) = \frac{\pi}{2} \left(\sin \tfrac{\pi}{2} t\right)^{r-1} \left(\cos \tfrac{\pi}{2} t\right)^{s-1} \frac{s\left(\sin \frac{\pi}{2} t\right)^2 + r\left(\cos \frac{\pi}{2} t\right)^2}{\left[\left(\sin \frac{\pi}{2} t\right)^r + \left(\cos \frac{\pi}{2} t\right)^s\right]^2}. \tag{2.15}$$

We will call $\phi_{r,s}(t)$ the $T^{r,s}$-transformation.

Clearly, when $r = s$, we have $u(t) = v(t)$, hence the $T^{r,r}$-transformation $\phi_{r,r}(t)$ is symmetric. We denote $\phi_{r,r}(t)$ by $\phi_r(t)$ for short and call it the T^r-transformation.

We use the $T^{r,s}$- and T^r-transformations in our numerical examples in Section 4.

3. ANALYSIS OF THE TRAPEZOIDAL RULE WITH CLASS $\mathcal{T}_{r,s}$ TRANSFORMATIONS

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

As always, 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 expansion due to the author (see, Sidi [11, Corollary 2.2]) as Theorem 3.1. 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 3.1. Let $u\in C^\infty(a,b)$, and assume that $u(x)$ has the asymptotic expansions

$$u\,(x)\sim\sum_{i=0}^{\infty}c_i\,(x-a)^{\gamma_i}\quad \text{as } x\to a+,$$
$$u\,(x)\sim\sum_{i=0}^{\infty}d_i\,(b-x)^{\delta_i}\quad \text{as } x\to b-,$$

where the γ_i and δ_i are distinct complex numbers that satisfy

$$-1<\Re\gamma_0\leqslant\Re\gamma_1\leqslant\Re\gamma_2\leqslant\cdots;\ \lim_{i\to\infty}\Re\gamma_i=+\infty,$$

$$-1<\Re\delta_0\leqslant\Re\delta_1\leqslant\Re\delta_2\leqslant\cdots;\ \lim_{i\to\infty}\Re\delta_i=+\infty.$$

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

$$h\sum_{i=1}^{n-1}u(a+ih)\sim\int_a^b u(x)\,dx+\sum_{\substack{i=0\\ \gamma_i\notin\{2,4,6,\ldots\}}}^{\infty}c_i\,\zeta(-\gamma_i)\,h^{\gamma_i+1}$$
$$+\sum_{\substack{i=0\\ \delta_i\notin\{2,4,6,\ldots\}}}^{\infty}d_i\,\zeta(-\delta_i)\,h^{\delta_i+1}\quad\text{as } h\to 0,$$

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

It is clear from Theorem 3.1 that even positive 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_i that is different from $2, 4, 6, \ldots$, and if δ_q is the first of the δ_i that is different from $2, 4, 6, \ldots$, then

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

Here is our main result:

Theorem 3.2. Let $f\in C^\infty(0,1)$, and assume that $f(x)$ has the asymptotic expansions

$$f(x)\sim\sum_{i=0}^{\infty}c_i x^{\gamma_i}\quad \text{as } x\to 0+;\quad f(x)\sim\sum_{i=0}^{\infty}d_i(1-x)^{\delta_i}\quad \text{as } x\to 1-.$$

Here γ_i and δ_i are distinct complex numbers that satisfy

$$-1<\Re\gamma_0\leqslant\Re\gamma_1\leqslant\Re\gamma_2\leqslant\cdots;\ \lim_{i\to\infty}\Re\gamma_i=+\infty,$$

$$-1<\Re\delta_0\leqslant\Re\delta_1\leqslant\Re\delta_2\leqslant\cdots;\ \lim_{i\to\infty}\Re\delta_i=+\infty.$$

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 us now make the transformation of variable $x=\phi(t)$ in $I[f]=\int_0^1 f(x)\,dx$, with $\phi\in\mathcal{T}_{r,s}$, the result of this being $I[f]=\int_0^1\widehat{f}(t)\,dt$, where $\widehat{f}(t)=f\big(\phi(t)\big)\phi'(t)$. Finally, let us approximate the transformed $I[f]$ via the trapezoidal rule $\widehat{Q}_n[f]=h\sum_{i=1}^{n-1}\widehat{f}(ih)$, where $h=1/n$, $n=1,2,\ldots$. Then the following hold:

(i) In the worst case,

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

(ii) If γ_0 and δ_0 are real, and if $r=(2k+1)/(\gamma_0+1)$ and $s=(2l+1)/(\delta_0+1)$, where k and l are positive integers, then, at worst,

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

where now

$$\omega = \min\{(\gamma_0 + 2)r,\ (\Re\gamma_1 + 1)r,\ (\delta_0 + 2)s,\ (\Re\delta_1 + 1)s\}.$$

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. To keep the presentation simple, we do the proof with $\phi(t)$ as in subsection 2.2. It is clear from Theorem 3.1 that we need to analyze the asymptotic expansions of the transformed integrand $\widehat{f}(t) = f\big(\phi(t)\big)\phi'(t)$ as $t \to 0$ and $t \to 1$. Because $\phi(t) \to 0$ as $t \to 0+$ and $\phi(t) \to 1$ as $t \to 1-$, we first have the genuine asymptotic expansions

$$\widehat{f}(t) \sim \sum_{i=0}^{\infty} K_i^{(0)}(t) \quad \text{as } t \to 0+; \quad K_i^{(0)}(t) = c_i[\phi(t)]^{\gamma_i}\phi'(t),$$

and

$$\widehat{f}(t) \sim \sum_{i=0}^{\infty} K_i^{(1)}(t) \quad \text{as } t \to 1-; \quad K_i^{(1)}(t) = d_i[1-\phi(t)]^{\delta_i}\phi'(t).$$

Invoking the relevant asymptotic expansions of $\phi(t)$ in subsection 2.2, and re-expanding, we have that $K_i^{(0)}(t)$ contributes the sum

$$\begin{aligned} K_i^{(0)}(t) &= \left[\sum_{k=1}^{\infty} R_{kr}(t)\right]^{\gamma_i} \sum_{k=1}^{\infty} R_{kr-1}(t) \quad \text{as } t \to 0+ \\ &= \sum_{k=1}^{\infty} R_{(\gamma_i+k)r-1}(t) \quad \text{as } t \to 0+, \end{aligned} \tag{3.1}$$

whereas $K_i^{(1)}(t)$ contributes the sum

$$\begin{aligned} K_i^{(1)}(t) &= \left[\sum_{k=1}^{\infty} R_{ks}(1-t)\right]^{\delta_i} \sum_{k=1}^{\infty} R_{ks-1}(1-t) \quad \text{as } t \to 1- \\ &= \sum_{k=1}^{\infty} R_{(\delta_i+k)s-1}(1-t) \quad \text{as } t \to 1-. \end{aligned} \tag{3.2}$$

To see this, we proceed as follows: As $z \to 0+$, and omitting the argument z in $R_p(z)$ (as $z \to 0+$), and taking $p > 0$ so that $R_p(z) = O(z^p) = o(1)$ as $z \to 0+$, there holds

$$\begin{aligned}
\left[\sum_{k=1}^{\infty} R_{kp}\right]^{\sigma} \sum_{k=1}^{\infty} R_{kp-1} &= \left[R_p\left(1+\sum_{k=1}^{\infty} R_{kp}\right)\right]^{\sigma}\left[R_{p-1}\left(1+\sum_{k=1}^{\infty} R_{kp}\right)\right] \\
&= \left[R_p^{\sigma}\left(1+\sum_{k=1}^{\infty} R_{kp}\right)^{\sigma}\right]\left[R_{p-1}\left(1+\sum_{k=1}^{\infty} R_{kp}\right)\right] \\
&= \left[R_{\sigma p}\left(1+\sum_{k=1}^{\infty} R_{kp}\right)\right]\left[R_{p-1}\left(1+\sum_{k=1}^{\infty} R_{kp}\right)\right] \\
&= R_{\sigma p} R_{p-1}\left(1+\sum_{k=1}^{\infty} R_{kp}\right)\left(1+\sum_{k=1}^{\infty} R_{kp}\right) \\
&= R_{\sigma p+p-1}\left(1+\sum_{k=1}^{\infty} R_{kp}\right) \\
&= \sum_{k=1}^{\infty} R_{(\sigma+k)p-1}.
\end{aligned}$$

We note that the most dominant terms in the asymptotic expansions of $\widehat{f}(t)$ as $t \to 0+$ and as $t \to 1-$ come from $K_0^{(0)}(t)$ and from $K_0^{(1)}(t)$, respectively, and they are $\alpha' t^{(\gamma_0+1)r-1}$ and $\beta'(1-t)^{(\delta_0+1)s-1}$, respectively, for some α' and β'. Thus, by Theorem 3.1, the most dominant terms in the expansion of $\widehat{Q}_n[f] - I[f]$ as $h \to 0$ are $\alpha h^{(\gamma_0+1)r}$ coming from the endpoint $t = 0$, and $\beta h^{(\delta_0+1)s}$ coming from the endpoint $t = 1$, for some α and β. This proves part (i) of the theorem.

To prove part (ii), we need a more refined study of the terms from $K_0^{(0)}(t)$ and from $K_0^{(1)}(t)$. The first term in the summation of (3.1), namely, $R_{(\gamma_0+1)r-1}(t)$, contains only even positive powers of t in its asymptotic expansion as $t \to 0+$ provided r is chosen such that $(\gamma_0+1)r = 2k+1$, where k is a positive integer. With this r, $R_{(\gamma_0+1)r-1}(t)$ contributes nothing to the Euler–Maclaurin expansion of $\widehat{Q}_n[f] - I[f]$ by Theorem 3.1. The most dominant terms that can contribute are (i) $R_{(\gamma_0+2)r-1}(t)$ of $K_0^{(0)}(t)$ and (ii) $R_{(\gamma_i+1)r-1}(t)$ of $K_i^{(0)}(t)$, $i \geqslant 1$, for which $\Re\gamma_i = \Re\gamma_1$. These terms contribute $\alpha h^{(\gamma_0+2)r}$ and $\beta_i h^{(\gamma_i+1)r}$, for some α and β_i.

Similarly, the first term in the summation of (3.2), namely, $R_{(\delta_0+1)r-1}(1-t)$, contains only even positive powers of $(1-t)$ in its asymptotic expansion as $t \to 1-$ provided s is chosen such that $(\delta_0+1)s = 2l+1$, where l is a positive integer. With this s, $R_{(\delta_0+1)s-1}(1-t)$ contributes nothing to the Euler–Maclaurin expansion of $\widehat{Q}_n[f] - I[f]$ by Theorem 3.1. The most dominant terms that can contribute are (i) $R_{(\delta_0+2)s-1}(1-t)$ of $K_0^{(1)}(t)$ and (ii) $R_{(\delta_i+1)s-1}(1-t)$ of $K_i^{(1)}(t)$, $i \geqslant 1$, for which $\Re\delta_i = \Re\delta_1$. These terms contribute $\alpha h^{(\delta_0+2)s}$ and $\beta_i h^{(\delta_i+1)s}$, for some α and β_i.

Combining the above, we complete the proof of the result in part (ii). □

Remark. Note that the result in part (ii) of Theorem 3.2 is made possible by our definition of the class $\mathcal{T}_{r,s}$ transformations, where we have excluded the powers t^{r+2i+1}, $i = 0, 1, \ldots, \lfloor r/2 \rfloor - 1$, and $(1-t)^{s+2i+1}$, $i = 0, 1, \ldots, \lfloor s/2 \rfloor - 1$, from the asymptotic expansions of $\phi(t)$ as $t \to 0+$ and $t \to 1-$.

Corollary 3.3. In case $f(x) = x^{\mu}(1-x)^{\nu} g(x)$, $g(x)$ being infinitely differentiable on [0, 1], the following hold:

(i) In the worst case,

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

(ii) If μ and ν are real, and if $r = (2k+1)/(\mu+1)$ and $s = (2l+1)/(\nu+1)$, where k and l are positive integers, then we have the optimal result

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

Corollary 3.4. When $\mu = \nu = c$, let $\phi \in \mathcal{T}_{r,r}$ in Corollary 3.3. Then the following hold:

(i) In the worst case,

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

(ii) If c is real, and if $r = (2k+1)/(c+1)$, where k is a positive integer, then we have the optimal result

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

In case $c = 0$ (that is, $f \in C^{\infty}[0.1]$) in Corollary 3.4, we have an error of $O(h^r)$ with arbitrary r, whereas the error is $O(h^{2r})$ when r is a positive odd integer, and this result is the same as that given in [9, Theorem 3.5] pertaining to class $\mathcal{S}_{r-1}$ variable transformations.

When $\mu \neq \nu$ in part (ii) of Corollary 3.3, we choose the integers k and l such that $(\mu+2)r \approx (\nu+2)s$, 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 $\widehat{f}(t) = f(\phi(t))\phi'(t)$ at the endpoints are of approximately the same strength.

3.1. An Improvement of the Numerical Quadrature Approximation to $I[f]$

In case $f(x) = x^{\mu}(1-x)^{\nu} g(x)$, with μ, ν real and > -1, $g \in C^{\infty}[0, 1]$, and g(0) and g(1) available, we can exploit the result of Corollary 3.3 to improve the accuracy of the approximation to $I[f]$ as follows: Let $v(x)$ be the linear function interpolating $g(x)$ at $x=0$ and $x=1$; that is, $v(x) = g(0) + [g(1) - g(0)]x$. Let also $g_0(x) = g(x) - v(x)$. Then

$$f(x) = p(x) + f_0(x); \quad p(x) = x^{\mu}(1-x)^{\nu} v(x), \quad f_0(x) = x^{\mu}(1-x)^{\nu} g_0(x),$$

and

$$I[f] = I[p] + I[f_0].$$

We now compute $I[p]$ exactly; we have

$$I[p] = g(0)B(\mu+1, \nu+1) + [g(1) - g(0)]B(\mu+2, \nu+1),$$

where $B(x, y)$ is the Beta function (see, for example, Abramowitz and Stegun [1, Formula 6.2.1]) that is given as in

$$B(x, y) = \int_0^1 \xi^{x-1}(1-\xi)^{y-1}\, d\xi = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)},$$

$\Gamma(z)$ being the Gamma function. Next, because $g_0(0) = g_0(1) = 0$, we have that $f_0(x)$ is now of the form $f_0(x) = x^{\mu+1}(1-x)^{\nu+1}\tilde{g}(x)$, $\tilde{g}(x)$ being a regular function on [0, 1]. In view of this, we apply the trapezoidal rule to the integral $I[f_0] = \int_0^1 \widehat{f_0}(t)\, dt$, where $\widehat{f_0}(t) = f_0(\phi(t))\phi'(t)$, where $\phi \in \mathcal{T}_{r,s}$ with $r = (2k+1)/(\mu+2)$ and $s = (2l+1)/(\nu+2)$, k and l being positive integers. Then, by Corollary 3.3, we have the optimal result

$$\left(I[p] + \widehat{Q}_n[f_0]\right) - I[f] = O\left(h^{\omega}\right) \quad \text{as } h \to 0; \quad \omega = \min\{(\mu+3)r, (\nu+3)s\}.$$

In case $\mu=\nu=c$, and $\phi\in\mathcal{T}_{r,r}$, with $r=(2k+1)/(c+2)$, where k is a positive integer, this result becomes,

$$\left(I[p]+\widehat{Q}_n[f_0]\right)-I[f]=O\left(h^{\omega}\right)\quad\text{as } h\to 0;\quad \omega=(c+3)r.$$

If, furthermore, $c=0$ [that is, $f\in C^{\infty}[0,1]$ and $g(x)=f(x)$], and $2r$ is a positive odd integer at least 3, then

$$\left(I[p]+\widehat{Q}_n[f_0]\right)-I[f]=O\left(h^{3r}\right)\quad\text{as } h\to 0.$$

4. NUMERICAL EXAMPLES

In this section, we provide two examples, considered already in [16], 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 4.1. Consider the integral

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

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 3.3, $\nu=0$ now.) Thus, if we choose r and s arbitrarily, we will obtain, by part (i) of Theorem 3.2 and Corollary 3.3,

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

In case $r=(2k+1)/(\mu+1)$ and $s=2l+1$, with k,l positive integers, we will obtain, by part (ii) of Theorem 3.2,

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

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 I, we give the relative errors in the $\widehat{Q}_n[f]$ for $n=2^k$, $k=1,\ldots,10$, obtained with the $T^{r,s}$-transformation. In column j of this table, we have chosen $r=(j+1.9)/(\mu+1)$ and $s=(j+1.9)/(\nu+1)$ when j is odd, while $r=(j+1)/(\mu+1)$ and $s=(j+1)/(\nu+1)$ when j is even. The superior convergence of the columns with j an even integer is clearly demonstrated. [Note that the r (the s), 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 II, we give the numbers

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

for the same values of r and s and for $k=1,2,\ldots,9$. It is seen that, with increasing k, the $\rho_{r,s,k}$ are tending to $\min\{(\mu+1)r,s\}$ when j an odd integer, and to $\min\{(\mu+2)r,2s\}$ when j is an even integer, completely in accordance with Theorem 3.2 and Corollary 3.3. (With the floating-point arithmetic we are using, this convergence seems to be less visible for relatively large r and s in the columns with even j.)

Example 4.2. Consider the integral

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

In this case, we have

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

where

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

If case $w(0)$ 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 r and s arbitrarily, we will obtain, by part (i) of Theorem 3.2 and Corollary 3.3,

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

In case $r=(2k+1)/(\mu+1)$ and $s=(2l+1)/(\nu+1)$, with k,l positive integers, we will obtain, by part (ii) of Theorem 3.2 and Corollary 3.3,

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

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

Table I. Errors in the Rules $\widehat{Q}_n[f]$ for the integral of Example 4.1 Obtained with $n=2^k$, $k=1(1)10$, and with the $T^{r,s}$-transformation

n	$j=1$	$j=2$	$j=3$	$j=4$	$j=5$	$j=6$	$j=7$	$j=8$	$j=9$	$j=10$
2	1.18*D*−01	1.57*D*−01	8.88*D*−01	9.26*D*−01	1.65*D*+00	1.69*D*+00	2.40*D*+00	2.44*D*+00	3.14*D*+00	3.17*D*+00
4	4.94*D*−04	1.26*D*−03	9.11*D*−02	1.01*D*−01	3.62*D*−01	3.78*D*−01	7.09*D*−01	7.27*D*−01	1.07*D*+00	1.09*D*+00
8	1.77*D*−04	3.41*D*−06	5.45*D*−04	6.88*D*−04	1.32*D*−02	1.46*D*−02	6.21*D*−02	6.57*D*−02	1.54*D*−01	1.59*D*−01
16	2.44*D*−05	6.33*D*−08	1.04*D*−07	1.27*D*−08	7.06*D*−06	8.83*D*−06	2.11*D*−04	2.40*D*−04	1.62*D*−03	1.75*D*−03
32	3.29*D*−06	1.14*D*−09	3.26*D*−09	2.26*D*−14	8.55*D*−12	1.21*D*−12	1.23*D*−09	1.62*D*−09	1.04*D*−07	1.24*D*−07
64	4.42*D*−07	2.03*D*−11	1.09*D*−10	2.83*D*−17	6.59*D*−14	1.62*D*−22	6.99*D*−17	2.96*D*−19	1.26*D*−15	1.80*D*−15
128	5.92*D*−08	3.64*D*−13	3.67*D*−12	3.56*D*−20	5.53*D*−16	1.43*D*−26	1.47*D*−19	1.29*D*−32	6.04*D*−23	1.87*D*−32
256	7.93*D*−09	6.57*D*−15	1.23*D*−13	4.52*D*−23	4.63*D*−18	1.28*D*−30	3.08*D*−22	0.00D+00	3.17*D*−26	1.93*D*−34
512	1.06*D*−09	1.19*D*−16	4.12*D*−15	5.81*D*−26	3.88*D*−20	9.63*D*−34	6.45*D*−25	3.85*D*−34	1.66*D*−29	5.78*D*−34
1024	1.42*D*−10	2.18*D*−18	1.38*D*−16	7.54*D*−29	3.25*D*−22	2.89*D*−34	1.35*D*−27	3.85*D*−34	7.90*D*−33	1.54*D*−33

In column j, we have chosen $r=(j+1.9)/(\mu+1)$ and $s=j+1.9$ when j is odd, while $r=(j+1)/(\mu+1)$ and $s=j+1$ when j is even.

Table II. The Numbers $\rho_{r,s,k} = \frac{1}{\log 2} \cdot \log\left(\frac{|\widehat{Q}_{2k}[f]-I[f]|}{|\widehat{Q}_{2k+1}[f]-I[f]|}\right)$, with $r, s, f(x)$, and $\widehat{Q}_n[f]$ as in Table I, 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	7.904	6.959	3.284	3.197	2.189	2.158	1.760	1.746	1.552	1.544
2	1.482	8.530	7.386	7.198	4.777	4.692	3.513	3.468	2.800	2.772
3	2.855	5.753	12.357	15.726	10.868	10.694	8.199	8.099	6.570	6.506
4	2.892	5.799	4.994	19.098	19.656	22.799	17.388	17.175	13.924	13.786
5	2.898	5.807	4.896	9.642	7.020	32.800	24.072	32.349	26.296	26.037
6	2.900	5.801	4.899	9.637	6.897	13.471	8.891	44.384	24.317	56.420
7	2.900	5.792	4.900	9.620	6.899	13.447	8.899	*	10.898	6.600
8	2.900	5.784	4.900	9.603	6.900	10.372	8.900	*	10.899	−1.585
9	2.900	5.776	4.900	9.589	6.900	1.737	8.900	0.000	11.036	−1.415
∞	2.9	5.727···	4.9	9.545···	6.9	13.363···	8.9	17.181···	10.9	21

In Table III, we give the absolute errors (recall that $I[f]=0$) in the $\widehat{Q}_n[f]$ for $n=2^k$, $k=1,\dots,10$, obtained with the $T^{r,s}$-transformation. In column j of this table, we have chosen $r=(j+1.9)/(\mu+1)$ and $s=(j+1.9)/(\nu+1)$ when j is odd, while $r=(j+1)/(\mu+1)$ and $s=(j+1)/(\nu+1)$ when j is even. The superior convergence of the columns with j an even integer is again clearly demonstrated. [Note that the r (the s), 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 IV, we give the numbers $\rho_{r,s,k}$ defined in the preceding example for the same values of r and s and for $k=1,2,\dots,9$. It is seen that, with increasing k, the $\rho_{r,s,k}$ are tending to $\min\{(\mu+1)r,(\nu+1)s\}$ when j an odd integer, and to $\min\{(\mu+2)r,(\nu+2)s\}$ when j is an even integer, completely in accordance with Theorem 3.2 and Corollary 3.3. (As in the preceding example, with the floating-point arithmetic we are using, this convergence seems to be less visible for relatively large r and s in the columns with even j.)

5. CONCLUDING REMARKS

In this work, we presented a class of variable transformations, which we denoted $\mathcal{T}_{r,s}$, whose members $\phi(t)$ have asymptotic expansions as $t\to 0+$ and $t\to 1-$ of the forms given in (2.4). We also noted that what gives these transformations their exceptional effectiveness is the fact that their asymptotic expansions include the powers t^{r+2i}, $i=0,1,\dots,\lfloor r/2\rfloor$, and $(1-t)^{s+2i}$, $i=0,1,\dots,\lfloor s/2\rfloor$, but exclude the powers t^{r+2i+1}, $i=0,1,\dots,\lfloor r/2\rfloor-1$, and $(1-t)^{s+2i+1}$, $i=0,1,\dots,\lfloor s/2\rfloor-1$. To see what happens if we do include the powers t^{r+2i+1}, $i=0,1,\dots,\lfloor r/2\rfloor-1$, and $(1-t)^{s+2i+1}$, $i=0,1,\dots,\lfloor s/2\rfloor-1$, let us modify the definition of class $\mathcal{T}_{r,s}$ by replacing the condition in (2.4) in Definition 2.1 by the following analogous condition:

$$
\begin{aligned}
\phi(t) &= \sum_{i=0}^{2\lfloor r/2\rfloor} \alpha_i t^{r+i} + O\big(t^{2r}\big) \quad \text{as } t\to 0+,\\
\phi(t) &= \sum_{i=0}^{2\lfloor s/2\rfloor} \beta_i (1-t)^{s+i} + O\big((1-t)^{2s}\big) \quad \text{as } t\to 1-,
\end{aligned}
\tag{5.1}
$$

which can be realized by taking, for example, $\phi(t)=t^r/[t^r+(1-t)^s]$, which is one of the variable transformations proposed in [7]. For convenience, let us denote by $\widetilde{\mathcal{T}}_{r,s}$ the resulting modification of class $\mathcal{T}_{r,s}$. With class $\widetilde{\mathcal{T}}_{r,s}$ variable transformations $\phi(t)$, the quality of the trapezoidal rule on

Table III. Errors in the Rules $\widehat{Q}_n[f]$ for the Integral of Example 4.2, Obtained with $n=2^k$, $k=1(1)10$, and with the $T^{r,s}$-transformation

n	$j=1$	$j=2$	$j=3$	$j=4$	$j=5$	$j=6$	$j=7$	$j=8$	$j=9$	$j=10$
2	9.10D−02	9.24D−02	9.23D−02	9.09D−02	3.94D−02	3.53D−02	6.63D−02	7.29D−02	2.19D−01	2.28D−01
4	2.50D−04	5.79D−05	2.44D−02	2.51D−02	1.50D−02	1.34D−02	3.40D−02	3.72D−02	1.10D−01	1.14D−01
8	3.58D−05	5.30D−06	1.62D−04	2.01D−04	1.06D−04	7.88D−05	1.18D−02	1.29D−02	4.36D−02	4.56D−02
16	5.69D−06	9.04D−08	2.35D−08	1.96D−10	4.38D−07	6.90D−07	9.45D−05	1.12D−04	1.22D−03	1.34D−03
32	7.82D−07	1.38D−09	7.79D−10	1.98D−13	1.88D−12	5.67D−15	1.48D−11	2.63D−11	8.07D−09	9.68D−09
64	1.05D−07	1.65D−11	2.61D−11	4.64D−16	1.57D−14	1.23D−20	1.68D−17	8.62D−23	5.50D−18	8.44D−18
128	1.41D−08	3.75D−14	8.74D−13	1.14D−18	1.32D−16	2.98D−24	3.51D−20	8.38D−30	1.44D−23	5.63D−36
256	1.89D−09	7.04D−15	2.93D−14	2.87D−21	1.10D−18	7.24D−28	7.34D−23	2.03D−34	7.54D−27	5.60D−35
512	2.53D−10	3.52D−16	9.80D−16	7.39D−24	9.23D−21	1.76D−31	1.54D−25	1.51D−35	3.95D−30	4.58D−35
1024	3.39D−11	1.29D−17	3.28D−17	1.92D−26	7.73D−23	1.21D−34	3.22D−28	1.60D−35	2.07D−33	5.77D−35

In column j, we have chosen $r=(j+1.9)/(\mu+1)$ and $s=(j+1.9)/(\nu+1)$ when j is odd, while $r=(j+1)/(\mu+1)$ and $s=(j+1)/(\nu+1)$ when j is even.

Table IV. The Numbers $\rho_{p,q,k} = \frac{1}{\log 2} \cdot \log\left(\frac{|\widehat{Q}_{2k}[f]-I[f]|}{|\widehat{Q}_{2k+1}[f]-I[f]|}\right)$, with $p, q, f(x)$, and $\widehat{Q}_n[f]$ as in Table III, 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	8.508	10.639	1.920	1.856	1.391	1.402	0.965	0.971	0.998	0.999
2	2.803	3.450	7.236	6.966	7.140	7.405	1.531	1.531	1.333	1.322
3	2.655	5.874	12.748	19.970	7.924	6.835	6.960	6.850	5.160	5.089
4	2.864	6.033	4.915	9.948	17.831	26.860	22.609	22.015	17.203	17.080
5	2.894	6.389	4.901	8.738	6.901	18.814	19.749	38.152	30.452	30.095
6	2.899	8.778	4.900	8.673	6.900	12.012	8.900	23.295	18.541	60.377
7	2.900	2.414	4.900	8.628	6.900	12.007	8.900	15.331	10.900	−3.314
8	2.900	4.321	4.900	8.602	6.900	12.003	8.900	3.752	10.900	0.290
9	2.900	4.776	4.900	8.587	6.900	10.510	8.900	−0.088	10.896	−0.331
∞	2.9	5.142···	4.9	8.571···	6.9	12	8.9	15.428···	10.9	18.857···

the transformed integrals $\int_0^1 f(\phi(t))\phi'(t)\,dt$ drops drastically. In particular, Corollary 3.3 and Corollary 3.4 assume the following forms:

Proposition 5.1. In case $f(x) = x^{\mu}(1-x)^{\nu}g(x)$, $g(x)$ being infinitely differentiable on [0, 1], the following hold:

(i) In the worst case,

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

(ii) If μ and ν are real, and if $r = (2k+1)/(\mu+1)$ and $s = (2l+1)/(\nu+1)$, where k and l are positive integers, then we have the optimal result

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

Proposition 5.2. When $\mu = \nu = c$, let $\phi \in \widetilde{\mathcal{T}}_{r,r}$ in Corollary 5.1. Then the following hold:

(i) In the worst case,

$$\widehat{Q}_n[f] - I[f] = O\big(h^{\omega}\big) \quad \text{as } h \to 0; \quad \omega = (\Re c + 1)r.$$

(ii) If c is real, and if $r = (2k+1)/(c+1)$, where k is a positive integer, then we have the optimal result

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

The proofs of these propositions are the same as those of Corollaries 3.3 and 3.4 and are left to the reader.

As can be seen by comparing parts (ii) of Corollaries 3.3 and 3.4 with parts (ii) of Propositions 5.1 and 5.2, the quality of $\widehat{Q}_n[f]$ drops with optimal values of r and s when we chose $\phi \in \widetilde{\mathcal{T}}_{r,s}$ since $r > 1$. That is, higher accuracy is achieved with class $\mathcal{T}_{r,s}$ transformations than with class $\widetilde{\mathcal{T}}_{r,s}$ transformations when r and s assume their optimal values. For example, if we let $c = 0$ so that $f \in C^{\infty}[0, 1]$, and take $r = s = 2k+1$ with k a positive integer, the error in $\widehat{Q}_n[f]$ is $O(h^{r+1})$ in Proposition 5.2, whereas it is $O(h^{2r})$ in Corollary 3.4.

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