# A NEW VARIABLE TRANSFORMATION FOR NUMERICAL INTEGRATION

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**Abstract**

Presently, variable transformations are used to enhance the performance of lattice rules for multidimensional integration. The transformations that are in the literature so far are of either polynomial or exponential nature. Following a short survey of some of the transformations that have been found to be effective, we propose a new transformation, denoted the $\sin^m$-transformation, that is neither polynomial nor exponential, but trigonometric, in nature. This transformation is also a representative of a general class of variable transformations that we denote $\mathcal{S}_m$. We analyze the effect of transformations in $\mathcal{S}_m$ within the framework of one-dimensional integration, and show that they have some very interesting and useful properties. Present results indicate that transformations in $\mathcal{S}_m$ can be more advantageous than known polynomial transformations, and have less underflow and overflow problems than exponential ones. Indeed, the various numerical tests performed with the $\sin^m$-transformation support this. We end the paper with numerical examples through which some of the theory is verified.

## 1 Introduction

Let $f(x)$ be a function defined on the interval $[0,1]$, and define

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

Let $Q_n[f]$ stand for either the trapezoidal rule $T_n[f]$ or the midpoint rule $M_n[f]$ for $I[f]$, which are given by

$$T_n[f] = \frac{1}{n}\left[\frac{1}{2}f(0) + \sum_{j=1}^{n-1} f\left(\frac{j}{n}\right) + \frac{1}{2}f(1)\right] \tag{1.2}$$

and

$$M_n[f] = \frac{1}{n}\sum_{j=1}^{n} f\left(\frac{j-1/2}{n}\right). \tag{1.3}$$

Then, provided $f(x)$ is differentiable on $[0,1]$ $2N+1$ times, we have the Euler-Maclaurin formula

$$I[f]-Q_n[f]=\sum_{\mu=1}^{N} c_\mu[f^{(2\mu-1)}(1)-f^{(2\mu-1)}(0)]n^{-2\mu}+R_N(n;f), \tag{1.4}$$

where

$$R_N(n;f)=O(n^{-2N-1}) \text{ as } n\to\infty. \tag{1.5}$$

The $c_\mu$ in (1.4) are constants independent of $f(x)$ and $n$, and are related to the Bernoulli numbers and polynomials. For details, see, e.g., Davis and Rabinowitz (1984).

In general, the error $I[f]-Q_n[f]$ is $O(n^{-2})$ as $n\to\infty$, by (1.4). When $f^{(2\mu-1)}(1)-f^{(2\mu-1)}(0)=0$, $1\le\mu\le k\le N-1$, it is obvious that $I[f]-Q_n[f]$ is $O(n^{-2k-2})$ as $n\to\infty$. This kind of an improvement can be achieved by a variable transformation of the form

$$I[f]=\int_0^1 f(\psi(t))\psi'(t)dt, \tag{1.6}$$

where $\psi(t)$ is an increasing function of $t$ on $[0,1]$ satisfying

$$\psi(0)=0 \text{ and } \psi(1)=1, \tag{1.7}$$

and has a sufficient number of derivatives that vanish at $t=0$ and $t=1$. Thus applying the trapezoidal rule or the midpoint rule to the integral on the right hand side of (1.6) results in very accurate approximations. For the sake of clarity we shall denote the trapezoidal and midpoint rule approximations on the transformed integral in (1.6) by $\hat{T}_n[f]$ and $\hat{M}_n[f]$, respectively, and let $\hat{Q}_n[f]$ stand for either one of them. We thus have

$$\hat{T}_n[f]=\frac{1}{n}\sum_{j=1}^{n-1} f\left(\psi\left(\frac{j}{n}\right)\right)\psi'\left(\frac{j}{n}\right) \tag{1.8}$$

and

$$\hat{M}_n[f]=\frac{1}{n}\sum_{j=1}^{n} f\left(\psi\left(\frac{j-1/2}{n}\right)\right)\psi'\left(\frac{j-1/2}{n}\right). \tag{1.9}$$

Comparing (1.8) with (1.2), we notice that the $j=0$ and $j=n$ terms in the former are missing. These two terms are automatically zero in (1.8) since $\psi'(0)=\psi'(1)=0$.

The idea of employing variable transformations seems to have been suggested first by Korobov (1963) in connection with the numerical approximation of integrals on the unit hypercube by lattice rules. The transformation of Korobov (1963) is a polynomial one, and is given by

$$\psi(t)=(2m+1)\binom{2m}{m}\int_0^t [u(1-u)]^m du. \tag{1.10}$$

Later Sag and Szekeres (1964) proposed the tanh-transformation

$$\psi(t) = \frac{1}{2}\tanh\left(-\frac{c}{2}\left(\frac{1}{t} - \frac{1}{1-t}\right)\right) + \frac{1}{2}, \quad c > 0. \tag{1.11}$$

(Actually, $c = 1$ in Sag and Szekeres(1964).) For this transformation

$$\psi^{(i)}(0) = \psi^{(i)}(1) = 0, \text{ all } i = 1, 2, \ldots . \tag{1.12}$$

In a historical paper Iri et al (1970) proposed the transformation

$$\psi(t) = \frac{\int_0^t \phi(u)du}{\int_0^1 \phi(u)du}, \tag{1.13}$$

where

$$\phi(t) = \exp\left(-\frac{c}{t(1-t)}\right) \text{ with } c > 0. \tag{1.14}$$

(Actually $c = 1$ in Iri et al (1970).) This has been known as the IMT-transformation in the literature. We note that (1.12) is satisfied by this transformation too.

We finally mention the double exponential transformation of Mori (1978), for which

$$\psi(t) = \frac{1}{2}\tanh\left(a\sinh\left(b\left(\frac{1}{1-t} - \frac{1}{t}\right)\right)\right) + \frac{1}{2}, \quad a, b > 0, \tag{1.15}$$

which also satisfies (1.12).

For a more complete list of references we refer the reader to the paper of Beckers and Haegemans (1991). In this paper the above mentioned transformations and a few others are compared with respect to their numerical efficiency when applied in conjunction with lattice rules (see, e.g., Sloan (1985) and Sloan and Kachoyan (1987)), to multiple integrals on the unit hypercube. One of the conclusions of this paper is that while polynomial transformations may be very well suited for well behaved integrands, IMT and tanh-transformations may be better for integrands with singularities on the boundary of the hypercube, although overflows and underflows may occur due to the fact that many of the abscissas may be extremely close to the surfaces of the hypercube because of the exponential nature of these transformations. (We also recall that a large number of the $\psi\left(\frac{j}{n}\right)$ and $\psi\left(\frac{j-1/2}{n}\right)$ in (1.8) and (1.9) are clustered in two very small regions, one to the right of 0 and the other to the left of 1, with quite a few of them being very close to 0 or 1. This may create overflow or underflow problems in some cases.)

In Section 2 of the present work we propose a new variable transformation $\psi(t)$ that is neither polynomial nor exponential, but trigonometric, in nature. This transformation is also a representative of a general class of variable transformations that we denote $\mathcal{S}_m$, and define properly again in Section 2. Any transformation $\psi(t)$ in $\mathcal{S}_m$, although not a polynomial itself, *behaves* polynomially at the end points $t = 0$ and $t = 1$, which ensures that the $\psi\left(\frac{j}{n}\right)$ and $\psi\left(\frac{j-1/2}{n}\right)$ in (1.8) and (1.9) cannot get too close to 0 or to 1, thus reducing the possibility of overflow and underflow. In Section 3 we analyze the effect of transformations in $\mathcal{S}_m$ in general, and of the $\sin^m$-transformation in particular, within the framework of one-dimensional integration of regular integrands. We do this by examining the Euler-Maclaurin expansions of the rules $\hat{Q}_n[f]$ in detail. It turns out that these expansions have a very surprising structure, and show that transformations in $\mathcal{S}_m$ are more effective than the analogous polynomial transformation of (1.10) in one-dimensional integration. (The sense of the analogy will be explained at the end of Section 2.) In Section 4 we provide a similar analysis for one-dimensional integrals of functions that have singularities at the end points of the integration interval. We have also observed numerically that the rules $\hat{Q}_n[f]$ with the $\sin^m$-transformation, when applied to both regular and singular integrals, produce results that compare very favorably with those obtained from IMT rules, despite the fact that the $\sin^m$-transformation does not satisfy (1.12). The approximations that were obtained for two such integrals are given in Section 5, and are seen to behave precisely as predicted by the results of Sections 3 and 4.

The results that we have obtained in this paper may suggest that variable transformations in $\mathcal{S}_m$ in general, and the $\sin^m$-transformation in particular, can be used very effectively in multiple integration in conjunction with lattice rules. We propose to study the theoretical and practical aspects of this usage in a future publication.

## 2 The $\sin^m$-Transformation

The $\sin^m$-transformation is defined by

$$\psi(t) = \frac{\Theta_m(t)}{\Theta_m(1)}, \tag{2.1}$$

where

$$\Theta_m(t) = \int_0^t (\sin \pi u)^m du, \quad m = 1, 2, \dots . \tag{2.2}$$

The recursion relation

$$\Theta_m(t) = -\frac{1}{\pi m}(\sin \pi t)^{m-1} \cos \pi t + \frac{m-1}{m}\Theta_{m-2}(t), \quad m = 2, 3, ..., \tag{2.3}$$

with the initial conditions

$$\Theta_0(t) = t \quad \text{and} \quad \Theta_1(t) = \frac{1}{\pi}(1 - \cos \pi t), \tag{2.4}$$

and the recursion relation

$$\Theta_m(1) = \frac{m-1}{m}\Theta_{m-2}(1), \quad m = 2, 3, ..., \tag{2.5}$$

with the initial conditions

$$\Theta_0(1) = 1 \quad \text{and} \quad \Theta_1(1) = \frac{2}{\pi}, \tag{2.6}$$

can be used to compute $\psi(t)$ for any $t$ in $(0,1)$ very efficiently and stably. It is easy to verify that $\Theta_m(1)$ can be expressed in terms of the beta function $B(\mu, \nu)$ as

$$\Theta_m(1) = \frac{2^m}{\pi} B\left(\frac{m+1}{2}, \frac{m+1}{2}\right) = \frac{2^m}{\pi} \frac{\left[\Gamma\left(\frac{m+1}{2}\right)\right]^2}{\Gamma(m+1)}. \tag{2.7}$$

Here is a short list of these transformations:

$$\begin{aligned}
\psi_1(t) &= \frac{1}{2}(1 - \cos \pi t) \\
\psi_2(t) &= \frac{1}{2\pi}(2\pi t - \sin 2\pi t) \\
\psi_3(t) &= \frac{1}{16}(8 - 9\cos \pi t + \cos 3\pi t) \\
\psi_4(t) &= \frac{1}{12\pi}(12\pi t - 8\sin 2\pi t + \sin 4\pi t)
\end{aligned}$$

## 2.1 A General Class of Variable Transformations

Now the $\sin^m$-transformation is a representative of a more general class of variable transformations that we shall denote $\mathcal{S}_m$. If $\psi(t)$ is in $\mathcal{S}_m$, then it has the following properties:

(a) $\psi \in C^\infty[0,1]$, increases on $[0,1]$, and satisfies $\psi(0) = 0$ and $\psi(1) = 1$.

(b) $\psi'(t)$ is symmetric with respect to $t = 1/2$, i.e., $\psi'(t) = \psi'(1-t)$. Consequently, $\psi(1-t) = 1 - \psi(t)$.

(c) $\psi'(t)$ has the asymptotic expansions

$$\begin{cases} \psi'(t) \sim \sum_{i=0}^{\infty} \epsilon_i t^{m+2i} & \text{as } t \to 0+ \\ \psi'(t) \sim \sum_{i=0}^{\infty} \epsilon_i (1-t)^{m+2i} & \text{as } t \to 1- . \end{cases} \tag{2.8}$$

where $\epsilon_0 > 0$. (Note that the second of the expansions in (2.8) is actually a consequence of the first and of property (b).)

By the nature of the function $\sin \pi t$ it is easy to show that the $\sin^m$-transformation possesses all three properties.

Note that all of the variable transformation $\psi(t)$ mentioned in Section 1 share properties (a) and (b). Property (c) implies that $\psi'(t) = O(t^m)$ as $t \to 0+$ and $\psi'(t) = O((1-t)^m)$ as $t \to 1-$ if $\psi \in \mathcal{S}_m$, and this is true also for the polynomial transformation of Korobov in (1.10). From this we conclude that, for $\psi \in \mathcal{S}_m$, the $\psi\left(\frac{j}{n}\right)$ and $\psi\left(\frac{j-1/2}{n}\right)$ will have the same kind of a distribution near the end points $t = 0$ and $t = 1$ as those of the Korobov transformation. It is in this sense that the $\sin^m$-transformation or any transformation in $\mathcal{S}_m$, and the Korobov transformation of (1.10) are analogous. It must be emphasized though that property (c) above is *not* shared by the Korobov transformation and is the most important and useful property of transformations in $\mathcal{S}_m$.

It would be interesting to know whether there are further variable transformations in $\mathcal{S}_m$ that can be expressed in terms of elementary functions as the $\sin^m$-transformation. So far we have not been successful in constructing such a transformation.

Before we close this section, we show that some kind of a "closure" property with respect to composition is satisfied by variable transformations in the classes $\mathcal{S}_m$, $m = 1, 2, \ldots$ .

**Lemma 2.1:** *Let $\psi_i \in \mathcal{S}_{m_i}$, $i = 1, 2, \ldots, r$, and define $\Psi = \psi_1 \circ \psi_2 \circ \cdots \circ \psi_r$ by $\Psi(t) = \psi_1(\psi_2(\cdots(\psi_r(t))\cdots))$. Then $\Psi \in \mathcal{S}_M$, with $M = \prod_{i=1}^{r}(m_i + 1) - 1$. Also $M$ is even if and only if all $m_i$ are even.*

**Proof:** The assertion follows from the definition of $\mathcal{S}_m$ for $r = 1$ and is easy to prove for $r = 2$. The result for general $r$ can be completed by induction. We leave the details to the reader. □

# 3 Euler-Maclaurin Expansions for Transformed Integrals of Regular Functions

Let the function $f(x)$ in (1.1) be differentiable on $[0, 1]$ as many times as needed. Let also $\psi(t)$ be a variable transformation in $\mathcal{S}_m$. In this section we will explore the properties of the Euler-Maclaurin expansions associated with the transformed integral (1.6). As the results for even $m$ are very different from those for odd $m$, we shall treat the two cases separately.

From the results below it will become clear that much better results are obtained for even $m$.

### 3.1 The Case $m$ =odd integer

**Theorem 3.1 :** *Let $m = 2k-1$ with $k$ a positive integer. Then, for $f \in C^{2p+1}[0,1]$, $p \geq k$, we have*

$$I[f] - \hat{Q}_n[f] = \sum_{\mu=k}^{p} c_\mu [F^{(2\mu-1)}(1) - F^{(2\mu-1)}(0)] n^{-2\mu} + O(n^{-2p-1}) \text{ as } n \to \infty, \tag{3.1}$$

*where $F(t) = f(\psi(t))\psi'(t)$ is the transformed integrand and $c_\mu$ are as in (1.4). Thus the error in $\hat{Q}_n[f]$ is at worst $O(n^{-m-1})$ as $n \to \infty$.*

**Proof:** Let us analyze the behavior of $F(t)$ for $t \to 0+$ and $t \to 1-$. Since $\psi'(t) = O(t^m)$ as $t \to 0+$ and $\psi'(t) = O((1-t)^m)$ as $t \to 1-$, and since $f(\psi(t)) \sim f(0)$ as $t \to 0+$ and $f(\psi(t)) \sim f(1)$ as $t \to 1-$, we have that $F(t) = O(t^m)$ as $t \to 0+$ and $F(t) = O((1-t)^m)$ as $t \to 1-$. Consequently, $F^{(i)}(0) = F^{(i)}(1) = 0$, $i = 1, 2, ..., m-1$. In addition, in general, $F^{(m)}(0) \neq 0$ and $F^{(m)}(1) \neq 0$. Since $m$ is odd and $f \in C^{2p+1}[0,1]$, (1.4) becomes (3.1). □

Let us now apply Theorem 3.1 to the constant function $f(x) = 1$. From the proof of this theorem it is easy to see that $I[f] - \hat{Q}_n[f] \sim -2(m!)c_k\epsilon_0 n^{-m-1}$ as $n \to \infty$ when $m = 2k-1$, $k \geq 1$. A much better result is obtained when $m$ is even, as we show in Lemmas 3.2 and 3.3 below.

### 3.2 The Case $m$ =even integer

**Lemma 3.2:** *Let $m$ be an even integer and let $f(x) = 1$. Then*

$$I[f] - \hat{Q}_n[f] = O(n^{-\mu}) \text{ as } n \to \infty, \text{ any } \mu > 0. \tag{3.2}$$

**Proof:** The transformed integrand now is simply $F(t) = \psi'(t)$. Since $m$ is even, the asymptotic expansions of $\psi'(t)$ for $t \to 0+$ and $t \to 1-$ contain only even powers of $t$ and $(1-t)$, respectively, as can be seen from (2.8). This implies that $F^{(2i-1)}(0) = F^{(2i-1)}(1) = 0$, $i = 1, 2, 3, \ldots$. Thus all the terms in the Euler-Maclaurin expansion vanish. This completes the proof. □

A substantial improvement results in Lemma 3.2 if the variable transformation $\psi \in \mathcal{S}_m$ is taken to be the $\sin^m$-transformation. This is considered in Lemma 3.3 below.

**Lemma 3.3:** *Let the variable transformation $\psi(t)$ in (1.6) be the $\sin^m$-transformation with $m = 2k,\ k \geq 1$, and let $f(x) = 1$. Then, provided $n > k$, we have*

$$\hat{Q}_n[f] = I[f]. \tag{3.3}$$

**Proof:** We start by observing that for $m = 2k$

$$\begin{aligned} \psi'(t) &= \frac{(\sin^2 \pi t)^k}{\Theta_m(1)} = \frac{(1-\cos 2\pi t)^k}{2^k \Theta_m(1)} \\ &= \sum_{j=0}^{k} \delta_j \cos 2\pi j t \quad \text{for some constants } \delta_j. \end{aligned} \tag{3.4}$$

That is to say, $\psi'(t)$ is a trigonometric polynomial of degree $k$ on $[0,1]$. Thus

$$\hat{Q}_n[f] = \sum_{j=0}^{k} \delta_j Q_n[\cos 2\pi j x], \tag{3.5}$$

where $Q_n$ stands for $T_n$ or $M_n$ depending on whether $\hat{Q}_n$ stands for $\hat{T}_n$ or $\hat{M}_n$, respectively. But

$$Q_n[\cos 2\pi j x] = I[\cos 2\pi j x] = \begin{cases} 1 & \text{if } j = 0, \\ 0 & \text{if } j \neq 0, \end{cases} \tag{3.6}$$

provided $n > j$. This completes the proof. □

**Corollary 3.4:** *The results of Lemmas 3.2 and 3.3 remain unchanged when $f(x) = A + Bx$, where $A$ and $B$ are constants.*

**Proof:** We can rewrite $f(x)$ in the form $f(x) = (A + B/2) + B(x - 1/2)$. From symmetry considerations, we have both $I[x-1/2] = 0$ and $\hat{Q}_n[x-1/2] = 0$. Thus $I[f] = (A+B/2)I[1]$ and $\hat{Q}_n[f] = (A + B/2)\hat{Q}_n[1]$. The result now follows by invoking Lemmas 3.2 and 3.3. □

**Note:** The result of Lemma 3.2 is very similar to the known analogous result for the IMT rules, in that in both cases the constant function is not integrated exactly, but the corresponding Euler-Maclaurin expansions are empty, suggesting rates of convergence that are better than $n^{-\mu}$ as $n \to \infty$ for any $\mu > 0$. The result of Lemma 3.3, however, says that the constant function is integrated exactly if $\psi(t)$ is the $\sin^m$-transformation with even $m$.

We now turn to the analysis of the Euler-Maclaurin expansion for arbitrary integrands $f(x)$ that are differentiable on $[0,1]$ as many times as needed. This expansion has a very interesting structure as we show in Theorem 3.5 below.

**Theorem 3.5:** *Let $m = 2k$ with $k$ a positive integer. Assume that $f \in C^{2p+1}[0,1]$ for $p \geq q(m+1)$, where $q$ is the smallest integer $\geq 1$ for which*

$$f^{(2q-1)}(1) - f^{(2q-1)}(0) \neq 0. \tag{3.7}$$

*Then*

$$I[f] - \hat{Q}_n[f] = \sum_{\mu=q(m+1)}^{p} c_\mu [F^{(2\mu-1)}(1) - F^{(2\mu-1)}(0)] n^{-2\mu} + O(n^{-2p-1}) \text{ as } n \to \infty, \tag{3.8}$$

*where $F(t) = f(\psi(t))\psi'(t)$ is the transformed integrand and $c_\mu$ are as in (1.4). Thus the error in $\hat{Q}_n[f]$ is $O(n^{-q(2m+2)})$ as $n \to \infty$.*

**Proof:** As in the proof of Theorem 3.1, we need to analyze the behavior of $F(t)$ for $t \to 0+$ and $t \to 1-$.

First, $f \in C^{2p+1}[0,1]$ implies that

$$f(x) = \sum_{j=0}^{2p} \frac{f^{(j)}(0)}{j!} x^j + O(x^{2p+1}) \text{ as } x \to 0+, \tag{3.9}$$

so that

$$F(t) = \psi'(t) \left\{ \sum_{j=0}^{2p} \frac{f^{(j)}(0)}{j!} [\psi(t)]^j + O([\psi(t)]^{2p+1}) \right\} \text{ as } t \to 0+\,. \tag{3.10}$$

Next, since $\psi \in \mathcal{S}_m$, we have from (2.8)

$$\psi(t) \sim \sum_{i=0}^{\infty} \frac{\epsilon_i}{m+2i+1} t^{m+2i+1} \text{ as } t \to 0+\,. \tag{3.11}$$

This, with $m = 2k$, implies that

$$\phi_j(t) \equiv \psi'(t)[\psi(t)]^j \sim t^{j(2k+1)+2k} \sum_{i=0}^{\infty} \epsilon_{ji} t^{2i} \text{ as } t \to 0+ \tag{3.12}$$

for some constants $\epsilon_{ji}$ with $\epsilon_{j0} > 0$. Thus the asymptotic expansion in (3.12) contains only even powers of $t$ when $j$ is even and only odd powers of $t$ when $j$ is odd. Since odd order derivatives of $t^{2\nu}$, $\nu = 0,1,2,\ldots$, are all zero at $t = 0$, we have $F^{(2j-1)}(0) = F_0^{(2j-1)}(0)$, where

$$F_0(t) = \psi'(t)\left\{\sum_{j=1}^{p} \frac{f^{(2j-1)}(0)}{(2j-1)!}[\psi(t)]^{2j-1} + O([\psi(t)]^{2p+1})\right\} \text{ as } t \to 0+. \tag{3.13}$$

Treating the other end point $t = 1$ similarly, we obtain $F^{(2j-1)}(1) = F_1^{(2j-1)}(1)$, where

$$F_1(t) = \psi'(1-t)\left\{\sum_{j=1}^{p} \frac{f^{(2j-1)}(1)}{(2j-1)!}[-\psi(1-t)]^{2j-1} + O([\psi(1-t)]^{2p+1})\right\} \text{ as } t \to 1-, \tag{3.14}$$

and we have invoked $\psi'(1-t) = \psi'(t)$ and $\psi(1-t) = 1 - \psi(t)$.

Since $\psi'(t)\psi(t) = \epsilon_{10}t^{4k+1} + O(t^{4k+3})$ as $t \to 0+$, we see that $F^{(i)}(0) = 0$, $i = 0,1,\ldots,4k$, but $F^{(4k+1)}(0) \neq 0$ in general. Similarly, $F^{(i)}(1) = 0$, $i = 0,1,\ldots,4k$, but $F^{(4k+1)}(1) \neq 0$ in general. This implies that the Euler-Maclaurin expansion is at worst $O(n^{-2m-2})$ as $n \to \infty$, and this is the result of (3.8) with $q = 1$ in (3.7).

To obtain the result for arbitrary $q \geq 1$ we need a more careful analysis of the odd order derivatives of $F(t)$ at $t = 0$ and $t = 1$.

From (3.13) and (3.14) we have

$$F^{(2\mu-1)}(1) - F^{(2\mu-1)}(0) = \sum_{j=1}^{p} \frac{f^{(2j-1)}(1) - f^{(2j-1)}(0)}{(2j-1)!}\phi_{2j-1}^{(2\mu-1)}(0), \quad \mu = 1,2,\ldots,p. \tag{3.15}$$

By (3.7), the summation on the right hand side of (3.15) actually begins with the term $j = q$. From (3.12),

$$\begin{aligned} \phi_{2j-1}^{(\nu)}(0) &= 0, \quad \nu = 0,1,\ldots,2j(2k+1)-2, \\ &\neq 0, \quad \nu = 2j(2k+1)-1. \end{aligned} \tag{3.16}$$

Consequently,

$$\begin{aligned} F^{(2\mu-1)}(1) - F^{(2\mu-1)}(0) &= 0, \quad \mu = 1,2,\ldots,q(2k+1)-1, \\ &\neq 0, \quad \mu = q(2k+1), \end{aligned} \tag{3.17}$$

and

$$F^{(2\mu-1)}(1) - F^{(2\mu-1)}(0) \propto f^{(2q-1)}(1) - f^{(2q-1)}(0) \text{ for } \mu = q(2k+1) = q(m+1). \tag{3.18}$$

The proof of the theorem can now be easily completed. □

**Remarks:**

1. It is very instructive to compare the results of Theorems 3.1 and 3.5. Under appropriate conditions on $f(x)$, we have for $\psi \in \mathcal{S}_m$

$$I[f] - \hat{Q}_n[f] = \begin{cases} O(n^{-m-1}) & \text{as } n \to \infty, \quad m \text{ odd}, \\ O(n^{-2m-2}) & \text{as } n \to \infty, \quad m \text{ even}, \end{cases} \tag{3.19}$$

in general, which shows the superiority of the transformations in $\mathcal{S}_m$ with even $m$.

2. It is also instructive to compare the errors in $\hat{Q}_n[f]$ obtained from a variable transformation $\psi \in \mathcal{S}_m$, namely, (3.19), with those obtained from the polynomial transformation $\psi$ of Korobov given in (1.10). For the latter it can easily be shown that

$$I[f] - \hat{Q}_n[f] = \begin{cases} O(n^{-m-1}) & \text{as } n \to \infty, \quad m \text{ odd}, \\ O(n^{-m-2}) & \text{as } n \to \infty, \quad m \text{ even}. \end{cases} \tag{3.20}$$

It is clear that also for the Korobov transformation better results are obtained for even $m$. In addition, transformations in $\mathcal{S}_m$ and the Korobov transformation produce the same rate of convergence for odd $m$, but the former are much better than the latter for even $m$.

# 4 Treatment of Transformed Integrals of Singular Functions

In the previous section we assumed that $f(x)$ was differentiable a sufficient number of times on $[0,1]$. We now turn to the case in which $f(x)$ is differentiable on $(0,1]$ a sufficient number of times, but has an algebraic singularity at $x = 0$ of the form $x^\alpha$, where $\alpha > -1$ is not an integer. We write the function $f(x)$ in the form

$$f(x) = x^\alpha g(x), \tag{4.1}$$

where we also assume that $g \in C^{2p+1}[0,1]$ and $g(0) \neq 0$.

By a result due to Navot (1961), the Euler-Maclaurin expansion of $I[f] - \hat{Q}_n[f]$ has different contributions coming from the end points $t = 0$ and $t = 1$ in the transformed integral (1.6). By taking $\psi \in \mathcal{S}_m$ in (1.6), we shall now give a brief analysis of these contributions.

First, we have

$$f(x)=\sum_{j=0}^{2p}\frac{g^{(j)}(0)}{j!}x^{j+\alpha}+O(x^{2p+\alpha+1})\ \text{ as } x\to 0+\,. \tag{4.2}$$

As a result, for some $a\neq 0,\ a\propto g(0)$,

$$F(t)\equiv f(\psi(t))\psi'(t)=at^{(m+1)\alpha+m}(1+O(t^2))\ \text{ as } t\to 0+\,. \tag{4.3}$$

Therefore, the dominant term in the contribution to the Euler-Maclaurin expansion of $I[f]-\hat{Q}_n[f]$ from $t=0$ is of the form $bn^{-(m+1)(\alpha+1)}$ at worst, for some $b\neq 0,\ b\propto g(0)$.

Next, we also have

$$f(x)=\sum_{j=0}^{2p}\frac{f^{(j)}(1)}{j!}(x-1)^j+O((x-1)^{2p+1})\ \text{ as } x\to 1-\,. \tag{4.4}$$

As a result,

$$F(t)=\sum_{j=0}^{2p}\frac{f^{(j)}(1)}{j!}[-\psi(1-t)]^j\psi'(1-t)+O([\psi(1-t)]^{2p+1}\psi'(1-t))\ \text{ as } t\to 1-\,. \tag{4.5}$$

Now the contribution from $t=1$ to the Euler-Maclaurin expansion of $I[f]-\hat{Q}_n[f]$ is of the form $\sum_{\mu=1}^{p}c_\mu F^{(2\mu-1)}(1)n^{-2\mu}$ with $c_\mu$ as before. From (4.5) and (2.8), we see that, for $p$ sufficiently large, the first odd order derivative of $F(t)$ that does not necessarily vanish at $t=1$ is $F^{(m)}(t)$ when $m$ is odd and $F^{(2m+1)}(t)$ when $m$ is even. This implies that the lower limit in the summation above is $\mu=\mu_0$, where $\mu_0\geq\bar{\mu}$ with $\bar{\mu}=(m+1)/2$ for odd $m$ and $\bar{\mu}=m+1$ for even $m$. Therefore, for $p$ sufficiently large, the contribution from $t=1$ to $I[f]-\hat{Q}_n[f]$ is at worst $O(n^{-2\bar{\mu}})$ as $n\to\infty$.

Finally, combining the different contributions from $t=0$ and $t=1$, we obtain

$$I[f]-\hat{Q}_n[f]=O(n^{-\omega})\ \text{ as } n\to\infty, \tag{4.6}$$

where

$$\omega=\begin{cases}\min((m+1)(\alpha+1),m+1), & m\text{ odd}\\ \min((m+1)(\alpha+1),2m+2), & m\text{ even,}\end{cases} \tag{4.7}$$

at worst.

The treatment above can easily be extended to functions $f(x)$ that are of the form $f(x)=x^\alpha(1-x)^\beta g(x)$, where $\alpha>-1$ and $\beta>-1$ are not integers, and $g(x)$ is differentiable on $[0,1]$ a sufficient number of times. In this case (4.6) holds with

$$\omega=\min((m+1)(\alpha+1),(m+1)(\beta+1)), \tag{4.8}$$

at worst. This result follows again from Navot (1961) and also from Lyness and Ninham (1967).

Similarly, we can treat the case in which $f(x)$ has logarithmic singularities at $x = 0$ or $x = 1$ or both, by using the results of Navot (1962). See also Lyness and Ninham (1967). We shall not pursue this matter further, however.

# 5 Numerical Examples

We have applied the transformed rules, namely $\hat{T}_n$ and $\hat{M}_n$, in conjunction with the $\sin^m$-transformations to various integrals, both regular and singular. The numerical results of our experiments provide ample verification for the theoretical results of this work and the conclusions that we have derived from them.

The numerical experiments reported in this section were done in extended precision arithmetic on an IBM-370 computer at the Computer Center of the Technion.

**Example 5.1:** $f(x) = e^x/(e+1)$.

$I[f] = (e-1)/(e+1)$ for this case. Table 5.1 shows the errors $|I[f] - \hat{T}_n[f]|$ obtained by employing the $\sin^m$-transformation, $m = 1, 2, ..., 8$, and $n = 2^s, s = 1, 2, ..., 10$. It is easy to verify that (3.19) is satisfied exactly. That is, the $m = 1, 2, ..., 8$ columns tend to zero like $n^{-2}, n^{-6}, n^{-4}, n^{-10}, n^{-6}, n^{-14}, n^{-8}, n^{-18}$, respectively. The last column shows the errors obtained by using the IMT rules with $c = 1$ in (1.14), and was taken from Table 3 in Iri et al (1970).

**Example 5.2:** $f(x) = \sqrt{x}$.

$I[f] = 2/3$ for this case. Table 5.2 shows that errors $|I[f] - \hat{T}_n[f]|$ obtained by employing the $\sin^m$-transformation, $m = 1, 2, ..., 8$, and $n = 2^s, s = 1, 2, ..., 10$. It is easy to verify that (4.7) is satisfied this time. That is, the $m = 1, 2, ..., 8$ columns tend to zero like $n^{-2}, n^{-4.5}, n^{-4}, n^{-7.5}, n^{-6}, n^{-10.5}, n^{-8}, n^{-13.5}$, respectively, by the fact that $\alpha = 1/2$. Again the last column shows the errors obtained by using the IMT rules with $c = 1$ in (1.14), and was taken from Table 3 in Iri et al (1970).

Table 5.1

| n \ m | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | IMT |
|---|---|---|---|---|---|---|---|---|---|
| 2 | 1.1D-01 | 1.9D-02 | 6.0D-02 | 1.3D-01 | 1.9D-01 | 2.5D-01 | 3.0D-01 | 3.5D-01 | 1.2D-01 |
| 4 | 2.6D-02 | 1.1D-04 | 2.1D-03 | 2.6D-03 | 6.9D-03 | 8.1D-03 | 5.7D-03 | 2.3D-04 | 4.0D-03 |
| 8 | 6.5D-03 | 9.9D-07 | 1.5D-04 | 2.0D-07 | 1.5D-05 | 1.8D-07 | 8.4D-06 | 4.9D-05 | 3.5D-05 |
| 16 | 1.6D-03 | 1.5D-08 | 9.4D-06 | 4.9D-11 | 2.2D-07 | 9.4D-13 | 1.1D-08 | 4.0D-12 | 3.5D-06 |
| 32 | 4.0D-04 | 2.2D-10 | 5.8D-07 | 4.3D-14 | 3.4D-09 | 4.8D-17 | 4.0D-11 | 1.9D-19 | 4.5D-09 |
| 64 | 1.0D-04 | 3.5D-12 | 3.6D-08 | 4.1D-17 | 5.2D-11 | 2.8D-21 | 1.5D-13 | 6.1D-25 | 3.2D-13 |
| 128 | 2.5D-05 | 5.4D-14 | 2.3D-09 | 4.0D-20 | 8.1D-13 | 1.7D-25 | 6.0D-16 | 2.2D-30 | 4.2D-18 |
| 256 | 6.3D-06 | 8.5D-16 | 1.4D-10 | 3.9D-23 | 1.3D-14 | 1.0D-29 | 2.3D-18 | 8.5D-33 | 4.0D-26 |
| 512 | 1.6D-06 | 1.3D-17 | 8.9D-12 | 3.8D-26 | 2.0D-16 | 9.6D-33 | 9.2D-21 | 9.6D-33 | |
| 1024 | 3.9D-07 | 2.1D-19 | 5.5D-13 | 3.7D-29 | 3.1D-18 | 6.6D-32 | 3.6D-23 | 6.5D-32 | |

Table 5.2

| n \ m | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | IMT |
|---|---|---|---|---|---|---|---|---|---|
| 2 | 1.1D-01 | 4.0D-02 | 1.7D-01 | 2.8D-01 | 3.7D-01 | 4.6D-01 | 5.5D-01 | 6.3D-01 | 1.0D-01 |
| 4 | 2.6D-02 | 6.1D-04 | 2.2D-03 | 6.3D-04 | 3.1D-03 | 1.1D-02 | 2.4D-02 | 4.2D-02 | 3.9D-03 |
| 8 | 6.5D-03 | 2.1D-05 | 1.5D-04 | 1.2D-06 | 1.6D-05 | 9.9D-08 | 4.1D-06 | 2.1D-06 | 1.4D-05 |
| 16 | 1.6D-03 | 8.8D-07 | 9.3D-06 | 5.1D-09 | 2.2D-07 | 1.1D-10 | 1.1D-08 | 7.0D-12 | 2.6D-07 |
| 32 | 4.0D-04 | 3.8D-08 | 5.8D-07 | 2.7D-11 | 3.4D-09 | 7.0D-14 | 4.0D-11 | 4.6D-16 | 1.4D-11 |
| 64 | 1.0D-04 | 1.7D-09 | 3.6D-08 | 1.5D-13 | 5.2D-11 | 4.7D-17 | 1.5D-13 | 3.7D-20 | 3.7D-16 |
| 128 | 2.5D-05 | 7.4D-11 | 2.3D-09 | 8.1D-16 | 8.1D-13 | 3.2D-20 | 6.0D-16 | 3.1D-24 | 1.4D-22 |
| 256 | 6.3D-06 | 3.3D-12 | 1.4D-10 | 4.5D-18 | 1.3D-14 | 2.2D-23 | 2.3D-18 | 2.7D-28 | 8.0D-32 |
| 512 | 1.6D-06 | 1.4D-13 | 8.9D-12 | 2.5D-20 | 2.0D-16 | 1.5D-26 | 9.2D-21 | 6.0D-32 | |
| 1024 | 3.9D-07 | 6.4D-15 | 5.5D-13 | 1.4D-22 | 3.1D-18 | 1.1D-29 | 3.6D-23 | 8.5D-32 | |

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