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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,