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Numerical integration of functions with boundary singularities ☆

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Abstract

In this paper we deal with the problem of constructing efficient rules for the numerical evaluation of integrals of functions which are very smooth everywhere in the domain of integration, except at the boundaries where they possess mild singularities. In particular, we consider integrals defined on bounded intervals or on triangles. Integrals of this type appear, for example, in the numerical solution of singular and weakly singular integral equations by boundary element methods. © 1999 Elsevier Science B.V. All rights reserved.

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1. Introduction

In several applications, in particular in the numerical solution of singular and weakly singular integral equations, one has to evaluate integrals of functions which are very smooth everywhere in the domain of integration, except at the boundaries of the latter where they possess mild singularities. This happens for instance when one has to solve one-dimensional integral equations by means of (collocation and Galerkin) boundary elements (see [1,6,10]). In these cases we may have to deal with integrals over bounded intervals, where the integrand functions $f(x)$ have endpoint singularities which can either be included into a weight function $w(x)$, such that $f(x)=w(x)g(x)$ with $g(x)$ smooth, or cannot be explicitly extracted.

A similar situation occurs in the numerical solution of two-dimensional singular and weakly singular integral equations by boundary element methods or in some finite element methods (see [15]).

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Indeed, in these cases, having subdivided the region of integration into triangles $\{T_i\}$ we may have to compute integrals of the form

$$\int_{T_i} w(x,y)g(x,y)\,\mathrm{d}x\,\mathrm{d}y \text{ or } \int_{T_i} f(x,y)\,\mathrm{d}x\,\mathrm{d}y,$$

where $w(x,y)$ or $f(x,y)$ is (weakly) singular at the boundary of T_i.

The numerical approach we present is not influenced by the presence or not of a weight function. Therefore, we will deal with the problem of constructing efficient rules for the numerical evaluation of integrals of the form

$$\int_a^b f(x)\,\mathrm{d}x, \tag{1.1}$$

and

$$\int_T f(x,y)\,\mathrm{d}x\,\mathrm{d}y, \tag{1.2}$$

where (a,b) is bounded, T is the reference triangle $0\leqslant x\leqslant 1$, $0\leqslant y\leqslant x$, and the integrand f has weak singularities at the boundaries of its domain of integration, but is smooth elsewhere.

Note that in the case of a function which has also interior singularities, for instance in (a,b), we can always subdivide (a,b) and go back to the above situation. Also in the case (1.2) this can often be done. Thus, in general, even if the singularities are located inside the domain of integration, we can often "confine" them to the boundaries of regions of integration by proper subdivisions of the latter.

The starting point for our work is that in many applications the location of the singularities is known a priori, and that an efficient quadrature rule should take this information into account.

To describe the numerical approach we propose, we will confine our presentation to integrals of type (1.1) where $f(x)$ has endpoint weak singularities, and, as an example of integration over triangles, with integrals of form (1.2) considered in [15,16], where

$$f(x,y) = y^{\lambda}(x-y)^{\mu}(1-x)^{\nu} r^{\beta} \log^k r\; g(x,y), \quad r=\sqrt{x^2+y^2}, \quad k=0,1, \tag{1.3}$$

$$\lambda,\mu,\nu > -1, \; \mu+\lambda+\beta > -2,$$

and $g(x,y)$ is assumed smooth. In this case, f has integrable singularities at the origin and along the edges of T. The application of our approach to other possible situations should then be straightforward.

Boundary singularities are less adverse than interior ones, from the point of view of the rate of convergence of the integration formulas that we will propose (see also [3,14,17]). Moreover, they can easily be weakened as much as we like by introducing proper smoothing changes of variable.

In the next section we will discuss some smoothing transformations that have recently been proposed.

In Sections 3 and 4 we will construct rules for the numerical evaluation of (1.1) and (1.2), respectively, and derive convergence results. Several numerical examples are presented, which show the efficiency of our rules.

2. Smoothing transformations

For simplicity, let us consider the case of the integral (1.1) where f has only endpoint singularities. If we introduce the change of variable $x=\varphi(t)$, with $\varphi'(t)\geqslant 0$, mapping (a,b) onto itself, we obtain

$$\int_a^b f(\varphi(t))\varphi'(t)\,\mathrm{d}t. \tag{2.1}$$

By choosing $\varphi(t)$ such that

$$\varphi^{(i)}(a)=0 \quad \text{and} \quad \varphi^{(j)}(b)=0, \quad i=1,\ldots,p-1, \quad j=1,\ldots,q-1,$$

we can make the integrand as smooth as we like and evaluate (2.1) by means of a Gaussian rule. In the following, for simplicity, we will refer to $(a,b)\equiv(0,1)$.

This very simple and natural smoothing approach is of course not new, but it has mainly been used with $p\equiv q$ to periodize the integrand in order to obtain high accuracy from the Trapezoidal rule (see [2,8,9,11–13,21–24]).

Here we propose to use Gaussian rules, namely Gauss–Legendre or (generalized) Gauss–Radau or Gauss–Lobatto formulas, since recent results (see [3,14,17]) show that when the singularities of the function f in (1.1) are at the endpoints of the interval of integration, the rates of convergence of these rules are more than twice those we have when the same singularities are located at interior points.

Several periodizing (smoothing in our context) functions have been proposed in the literature. They are of polynomial, trigonometric, rational or exponential type. Here we recall those we think are the most relevant ones.

In [19] (see also [20]), the following polynomial transformation, which is a generalization of the one proposed in [12] to construct lattice rules for multiple integration on the hypercube, has been used

$$\varphi_1(t)=\frac{(p+q-1)!}{(p-1)!(q-1)!}\int_0^t u^{p-1}\,(1-u)^{q-1}\,\mathrm{d}u, \quad p,q\geqslant 1. \tag{2.2}$$

The integrals

$$\Psi_{p,q}(t):=\int_0^t u^{p-1}(1-u)^{q-1}\,\mathrm{d}u, \quad p,q\geqslant 1$$

could be computed, for any $t\in(0,1]$, using the following recurrence relations:

$$\Psi_{p,q}(t)=\frac{1}{p+q-1}[t^p(1-t)^{q-1}+(q-1)\Psi_{p,q-1}(t)], \quad p\geqslant 1,\ q\geqslant 2,$$

$$\Psi_{p,q}(t)=\frac{1}{p+q-1}[-t^{p-1}(1-t)^q+(p-1)\Psi_{p-1,q}(t)], \quad p\geqslant 2,\ q\geqslant 1$$

with the following starting value:

$$\Psi_{1,1}(t)=t.$$

Numerical testing shows, however, that when t is very small the second of these relations is unstable; in any case $\Psi_{p,q}(t)$ can be evaluated more efficiently, for the given values of p and q, by means of the n-point Gauss–Legendre rule, with $n=\lfloor (p+q)/2\rfloor$.[1]

A trigonometric transformation of the form

$$\varphi(t)=\frac{\int_0^t(\sin\pi u)^{p-1}\,\mathrm{d}u}{\int_0^1(\sin\pi u)^{p-1}\,\mathrm{d}u},\quad p\geqslant 1,$$

has been proposed and examined in [24], and a recursive procedure to evaluate it for the chosen value of p has also been derived. Incidentally, we note that $\varphi(t)$ can be generalized to allow for a different smoothing degree at the endpoints:

$$\varphi_2(t)=\frac{\int_0^t(\sin\frac{\pi}{2}u)^{p-1}\left(\cos\frac{\pi}{2}u\right)^{q-1}\,\mathrm{d}u}{\int_0^1\left(\sin\frac{\pi}{2}u\right)^{p-1}\left(\cos\frac{\pi}{2}u\right)^{q-1}\,\mathrm{d}u},\quad p,q\geqslant 1. \tag{2.3}$$

The integrals

$$\Theta_{p,q}(t):=\int_0^t\left(\sin\frac{\pi}{2}u\right)^{p-1}\left(\cos\frac{\pi}{2}u\right)^{q-1}\,\mathrm{d}u,\quad p,q\geqslant 1,$$

in (2.3) could be computed for any $t\in(0,1]$ by using the following recurrence relations in a proper way:

$$\Theta_{p,p}(t)=-\frac{2^{1-p}}{\pi(p-1)}(\sin\pi t)^{p-2}\cos\pi t+\frac{p-2}{4(p-1)}\Theta_{p-2,p-2}(t),$$

when $p\equiv q,\ p\geqslant 3$, and

$$\begin{aligned}\Theta_{p,q}(t)&=\frac{2}{\pi(p+q-2)}\left(\sin\frac{\pi}{2}t\right)^{p}\left(\cos\frac{\pi}{2}t\right)^{q-2}+\frac{q-2}{p+q-2}\Theta_{p,q-2}(t),\quad p\geqslant 1,\quad q\geqslant 3,\\ \Theta_{p,q}(t)&=-\frac{2}{\pi(p+q-2)}\left(\sin\frac{\pi}{2}t\right)^{p-2}\left(\cos\frac{\pi}{2}t\right)^{q}+\frac{p-2}{p+q-2}\Theta_{p-2,q}(t),\quad p\geqslant 3,\quad q\geqslant 1,\end{aligned} \tag{2.4}$$

when $p\neq q$. The starting values are

$$\Theta_{1,1}(t)=t,\quad \Theta_{2,1}(t)=\frac{2}{\pi}\left(1-\cos\frac{\pi}{2}t\right),$$

$$\Theta_{1,2}(t)=\frac{2}{\pi}\sin\frac{\pi}{2}t,\quad \Theta_{2,2}(t)=\frac{1}{2\pi}(1-\cos\pi t).$$

However, also the second relation in (2.4) seems to be unstable when t is close to zero. In such a situation, a direct computation of $\Theta_{p,q}$ using a Gauss rule, as in the case of $\varphi_1(t)$, appears more efficient, particularly when p,q are not small.

[1] Or the $(n+1)$-point Gauss–Radau rule, with $n=\lfloor (p+q-1)/2\rfloor$, when $p>1$ ($\lfloor x\rfloor$= the greatest integer less than or equal to x).

A third transformation, of rational type, used in [8,22] in connection with the solution of certain integral equations, and in [9] to evaluate Hadamard finite-part integrals, is the following one:

$$\varphi(t) = \frac{t^p}{t^p + (1-t)^p}.$$

Also this transformation can be easily generalized to the nonsymmetric case in order to have $p-1$ and $q-1$ first derivatives vanishing at 0 and 1, respectively. We have

$$\varphi_3(t) = \frac{t^p}{t^p + (1-t)^q}, \quad p, q \geqslant 1. \tag{2.5}$$

The last transformations we consider are of exponential type:

$$\varphi_4(t) = \frac{\int_0^t e^{-c/u(1-u)}\, du}{\int_0^1 e^{-c/u(1-u)}\, du}, \quad c > 0,$$

$$\varphi_5(t) = \tfrac{1}{2} + \tfrac{1}{2}\tanh\left(\gamma \sin h \left(\sigma \left(\frac{1}{1-t} - \frac{1}{t}\right)\right)\right), \quad \gamma, \sigma > 0.$$

They are known as the IMT-transformation (see [11,4]) and the double exponential transformation (see [21,4]), respectively. The first cannot be evaluated directly but needs to be approximated by some truncated expansion (see [5]); the second is an alternative which does not require as much work for its computation (see also [23]). They both have the property of having all derivatives vanish at the endpoints; but unfortunately, they also have the drawback of concentrating many quadrature nodes too close to the endpoints. Moreover, the parameters c, γ, σ must be chosen very carefully since they affect the efficiency of the transformations considerably. Although in some specific applications these transformations have been shown to be quite efficient (see [6]), we will not consider them in the following, because of the above reasons.

3. Integrals on bounded intervals

Also in this section, for simplicity, we refer to the interval of integration $(0,1)$. First, we compare the first three changes of variable presented in Section 2, by introducing them into (1.1) and evaluating the corresponding new form (2.1) by a Gauss-type rule. Only $\varphi_2(t)$ has been computed using the corresponding recurrence relations. In particular, this has been done in the examples reported in the first three tables, since the values of p, q are very small and instability did not show up yet. In Table 4 we have not used $\varphi_2(t)$ because its accurate evaluation, particularly when t is small, appears more expensive than that of $\varphi_1(t)$ or of $\varphi_3(t)$.

Extensive testing has shown that the nonsymmetric transformation are the most efficient ones for our purposes. Moreover, when p, q are very small, we have noticed very minor differences between $\varphi_1(t)$, $\varphi_2(t)$ and $\varphi_3(t)$; nevertheless, we have preferred $\varphi_1(t)$. A sample of comparisons between the performances given by the n-point Gauss–Legendre quadrature rule, after having introduced these transformations, is reported in Tables 1–4.

Incidentally we note that, particularly when the number of nodes n is fixed and very small, by increasing the smoothing exponents the accuracy produced by the quadrature rule may not improve

Table 1
Gauss–Legendre absolute errors obtained with φ_i, $i=1,2,3$ when $f(x)=\log x$

	p	q	$n=2$	$n=4$	$n=8$	$n=16$	$n=32$	$n=64$	$n=128$
φ_1	2	1	3.14E−02	2.60E−03	1.96E−04	1.36E−05	9.01E−07	5.81E−09	3.68E−09
	3	1	2.31E−02	4.27E−04	8.28E−06	1.49E−07	2.54E−09	4.14E−11	6.63E−13
	4	1	4.90E−02	1.26E−04	5.83E−07	2.68E−09	1.16E−11	4.84E−14	—[a]
	5	1	1.87E−01	6.43E−05	6.32E−08	7.21E−11	7.85E−14	—	—
φ_2	2	1	3.71E−02	3.19E−03	2.41E−04	1.68E−05	1.11E−06	7.16E−08	4.55E−09
	3	1	8.75E−02	6.91E−04	1.36E−05	2.46E−07	4.17E−09	6.81E−11	1.09E−12
	4	1	1.44E−01	1.96E−04	1.32E−06	6.12E−09	2.65E−11	1.09E−13	—
	5	1	1.09E−01	1.54E−03	2.00E−07	2.34E−10	2.56E−13	—	—
φ_3	2	1	2.93E−03	2.33E−03	1.90E−04	1.35E−05	9.00E−07	5.80E−08	3.68E−09
	3	1	2.77E−01	1.07E−02	4.83E−06	1.47E−07	2.53E−09	4.14E−11	6.63E−13
	4	1	3.60E−01	2.48E−03	7.23E−05	3.21E−09	1.15E−11	4.73E−14	—
	5	1	2.46E−01	6.03E−02	4.54E−04	1.45E−08	7.79E−14	—	—

[a]Here and in the tables below the symbol — means that the corresponding approximation has achieved full accuracy, i.e., 14 significant digits in our case.

Table 2
Gauss–Legendre absolute errors obtained with φ_i, $i=1,2,3$ when $f(x)=2x\log x+(1-x)\log(1-x)$

	p	q	$n=2$	$n=4$	$n=8$	$n=16$	$n=32$	$n=64$	$n=128$
φ_1	2	2	2.14E−01	1.29E−03	4.41E−06	1.86E−08	7.89E−11	3.25E−13	—
	3	3	4.43E−01	2.10E−02	1.43E−06	2.35E−10	5.77E−14	—	—
	4	4	5.86E−01	7.92E−02	2.03E−06	1.26E−11	—	—	—
	5	5	6.66E−01	1.54E−01	9.21E−05	3.70E−12	—	—	—
φ_2	2	2	2.59E−01	1.46E−03	2.62E−06	1.22E−08	5.29E−11	2.19E−13	—
	3	3	5.01E−01	4.33E−02	1.15E−06	8.81E−11	2.42E−14	—	—
	4	4	6.34E−01	1.26E−01	1.08E−04	2.28E−12	—	—	—
	5	5	6.99E−01	2.20E−01	1.17E−03	4.06E−13	—	—	—
φ_3	2	2	4.74E−01	6.05E−02	2.31E−04	1.09E−09	8.51E−12	3.59E−14	—
	3	3	7.03E−01	3.20E−01	1.73E−02	1.18E−05	1.20E−12	—	—
	4	4	7.44E−01	5.51E−01	9.56E−02	6.78E−04	7.54E−09	—	—
	5	5	7.49E−01	6.72E−01	2.27E−01	6.15E−03	1.01E−06	—	—

at all or even become worse. This is due to the increasing flatness of the new integrand function around the singular points.

Our approach has been strongly suggested by the following convergence results, which refer to the use of a n-point Gauss–Legendre (or $(n+1)$-point Gauss–Radau or $(n+2)$-point Gauss–Lobatto) quadrature formula:

$$\int_0^1 f(x)\,\mathrm{d}x=\delta_{1,j}w_0 f(0)+\sum_{i=1}^{n} w_{n,i}f(x_{n,i})+\delta_{1,l}w_{n+1}f(1)+R_n(j,l;f), \tag{3.1}$$

where $\delta_{r,s}$ denotes the Kronecker symbol, $j,l\in\{0,1\}$.

Table 3
Gauss–Legendre absolute errors obtained with φ_i, $i = 1, 2, 3$ when $f(x) = x^{-1/5}$

	p	q	$n=2$	$n=4$	$n=8$	$n=16$	$n=32$	$n=64$	$n=128$
φ_1	2	1	1.08E−02	1.52E−03	1.94E−04	2.31E−05	2.63E−06	2.93E−07	3.23E−08
	3	1	3.93E−03	1.84E−04	8.13E−06	3.31E−07	1.27E−08	4.73E−10	1.73E−11
	4	1	1.78E−03	2.34E−05	3.43E−07	4.71E−09	6.09E−11	7.57E−13	1.22E−14
	5	1	—	—	—	—	—	—	—
φ_2	2	1	1.13E−02	1.79E−03	2.29E−04	2.73E−05	3.11E−06	3.47E−07	3.82E−08
	3	1	1.22E−02	2.71E−04	1.21E−05	4.92E−07	1.89E−08	7.04E−10	2.57E−11
	4	1	1.68E−03	4.27E−05	6.61E−07	9.12E−09	1.18E−10	1.43E−12	3.95E−14
	5	1	4.27E−02	7.96E−05	1.04E−12	—	—	—	—
φ_3	2	1	3.21E−02	1.08E−03	1.91E−04	2.30E−05	2.63E−06	2.93E−07	3.23E−08
	3	1	6.57E−02	1.85E−03	5.21E−06	3.28E−07	1.27E−08	4.72E−10	1.73E−11
	4	1	5.60E−02	1.82E−02	3.90E−05	4.61E−09	6.07E−11	7.55E−13	—
	5	1	2.67E−01	2.94E−02	1.12E−04	4.02E−10	—	—	—

Table 4
Gauss–Legendre absolute errors obtained with φ_i, $i = 1, 3$ when $f(x) = x^{-0.91}$

	p	q	$n=2$	$n=4$	$n=8$	$n=16$	$n=32$	$n=64$	$n=128$
φ_1	8	1	6.55E−01	2.79E−01	1.11E−01	4.28E−02	1.61E−02	6.01E−03	2.23E−03
	11	1	1.19E−02	3.63E−03	1.03E−03	2.75E−04	7.19E−05	1.85E−05	4.72E−06
	17	1	1.13E−01	1.75E−02	2.45E−03	3.20E−04	4.02E−05	4.93E−06	5.99E−07
	20	1	4.29E−02	4.65E−03	4.56E−04	4.15E−05	3.61E−06	3.06E−07	2.56E−08
	25	1	2.97E−02	1.73E−03	9.35E−05	4.65E−06	2.19E−07	1.00E−08	4.50E−10
	35	1	1.22E−02	1.75E−04	2.75E−06	4.05E−08	5.60E−10	7.46E−12	1.24E−13
	50	1	1.11E−01	6.61E−05	1.44E−07	3.30E−10	6.70E−13	2.13E−14	4.44E−14
φ_3	8	1	5.63E−01	2.16E−01	1.10E−01	4.28E−02	1.61E−02	6.00E−03	2.23E−03
	11	1	8.70E−01	6.31E−02	1.76E−03	2.70E−04	7.19E−05	1.85E−05	4.72E−06
	17	1	2.39E+00	5.09E−01	3.25E−02	2.21E−04	4.02E−05	4.93E−06	5.98E−07
	20	1	2.68E+00	7.05E−01	3.89E−02	2.50E−04	3.61E−06	3.06E−07	2.56E−08
	25	1	2.85E+00	8.41E−01	2.44E−02	8.65E−04	1.35E−07	1.00E−08	4.50E−10
	35	1	2.88E+00	3.86E−01	2.53E−01	6.24E−03	2.77E−06	7.88E−12	1.24E−13
	50	1	2.46E+00	1.44E+00	1.75E−01	2.18E−02	4.07E−05	7.00E−11	6.22E−14

Theorem 1 (see Monegato [18]). *Let $f(x) = x^m \log^k x$, with $m \geqslant k$ positive integers. Then we have*

$$R_n(0,0;f) = \mathrm{O}(n^{-2m-2+\varepsilon}), \tag{3.2}$$

with $\varepsilon > 0$ arbitrarily small.

Remark 1. For $k = 1$ we actually have (see [3]) the sharper bound $\mathrm{O}(n^{-2m-2} \log n)$.

Theorem 2 (see Küntz [14]). *Let* $f(x)=x^\sigma, \sigma$ *not an integer, with* $\sigma > -1$ *if in* (3.1) *we set* $j=l=0$ *and* $\sigma > 0$ *if in* (3.1) $j=1$. *Then we have*

$$R_n(j,l;f) = \mathrm{O}(n^{-2\sigma-2}). \tag{3.3}$$

These first two theorems are useful when, for instance, it is known a priori that the integrand function admits an expansion whose terms are of the form $x^\sigma((1-x)^\sigma)$, $x^m \log^k x((1-x)^m \log^k(1-x))$, with σ not an integer.

Similar error bounds have been also derived in [17] for functions which do not admit expansions of the above type, but nevertheless belong to one of the sets

$$C_\sigma^m[0,1] := \{f \in L_1(0,1) : x^{i-\sigma} f^{(i)}(x) \in C[0,1], \quad i=0,\ldots,m\},$$

$$\bar{C}_\sigma^m[0,1] := \{f \in L_1(0,1) : [x(1-x)]^{i-\sigma} f^{(i)}(x) \in C[0,1], \quad i=0,\ldots,m\}.$$

They are recalled in the next two theorems, where we have defined

$$\Phi(x) := x^{m-\sigma} f(x), \quad f \in C_\sigma^m[0,1],$$

$$\bar{\Phi}(x) := [x(1-x)]^{m-\sigma} f(x), \quad f \in \bar{C}_\sigma^m[0,1],$$

$$E_m(f) = \min_{p_m \in \Pi_m} \|f - p_m\|_\infty,$$

Π_m being the space of algebraic polynomials of degree m.

Theorem 3. *Let* $f(x) \in C_\sigma^m[0,1]$, *with* $\sigma \geqslant 0$ and $m > 2\sigma + 2$. *Then we have*

$$|R_n(0,l;f)| \leqslant c \, \frac{\log n}{n^{2\sigma+2}} \, E_{n-m-1}(\Phi^{(m)}), \tag{3.4}$$

with a constant c independent of n and f.

Proof. Estimate (3.4) follows from the results obtained in [17].

Theorem 4 (see Mastroianni [17]).[2] *Let* $f(x) \in \bar{C}_\sigma^m[0,1]$, *with* $\sigma \geqslant 0$ *and* $m > 2\sigma + 2$. *Then we have*

$$|R_n(0,0;f)| \leqslant c \, \frac{\log n}{n^{2\sigma+2}} \, E_{n-m-1}(\bar{\Phi}^{(m)}), \tag{3.5}$$

with a constant c independent of n and f.

One of the main advantages of our approach is that we need to regularize the integrand only at the endpoints where it is singular. Furthermore, the smoothing exponent does not need to be the same at each endpoint; actually it needs to be the smallest one which guarantees the required degree of smoothness. This is important since the higher the exponent, the higher the concentration of quadrature nodes produced by the transformation near the corresponding endpoint.

When the transformation $\varphi(t)$ is used to periodize the integrand, in order to obtain high accuracy using the Trapezoidal rule, the number of vanishing derivatives must generally be the same at both

[2] Notice that Theorems 4 and 5 in [17] trivially hold also when there we assume $v = 0$.

Table 5
Absolute errors obtained by Gauss–Legendre (with φ_1) and Trapezoidal (with φ_3) rules when $f(x)=\log x$

	p	q	$n=2$	$n=4$	$n=8$	$n=16$	$n=32$	$n=64$	$n=128$
φ_1	2	1	3.14E−02	2.60E−03	1.96E−04	1.36E−05	9.01E−07	5.81E−08	3.68E−09
and	3	1	2.31E−02	4.27E−04	8.28E−06	1.49E−07	2.54E−09	4.14E−11	6.63E−13
G.L.	4	1	4.90E−02	1.26E−04	5.83E−07	2.68E−09	1.16E−11	4.84E−14	—
	5	1	1.87E−01	6.43E−05	6.32E−08	7.21E−11	7.85E−14	—	—
φ_3	2	2	1.20E−01	5.05E−02	1.77E−02	5.63E−03	1.69E−03	4.87E−04	1.37E−04
and	3	3	2.89E−02	3.01E−03	2.38E−04	4.37E−05	6.62E−06	9.20E−07	1.22E−07
T.	4	4	3.87E−02	1.78E−02	4.87E−04	5.93E−06	4.80E−07	3.65E−08	2.67E−09
	5	5	2.23E−01	1.68E−02	2.87E−03	2.98E−06	3.44E−09	1.39E−10	4.96E−12

endpoints. But this also means that we will unnecessarily concentrate quadrature nodes near an endpoint where the function is, for instance, smooth.

Another important advantage of our approach is its rate of convergence, which is more than twice that produced, for example, by the use of the corresponding symmetric version of the transformation $\varphi_2(t)$ combined with the Trapezoidal rule (see [24]). Indeed, for example, for functions of form

$$f(x)=\begin{cases} x^\sigma g(x),\ g(x) \text{ smooth with } g(0)\neq 0, \\ x^\sigma(1-x)^\gamma g(x), \quad g(x) \text{ smooth with } g(0)\neq 0, \quad g(1)\neq 0, \end{cases}$$

where we assume $\sigma,\gamma>-1$, by taking exponents $p=q=m+1$ in $\varphi_2(t)$, an error estimate of type $O(n^{-\omega})$ was derived in [24], where

$$\omega=\min\{(m+1)(\sigma+1),\ m+1\}, \quad m \text{ odd},$$
$$\omega=\min\{(m+1)(\sigma+1),\ 2m+2\}, \quad m \text{ even},$$

in the first case, and

$$\omega=\min\{(m+1)(\sigma+1),\ (m+1)(\gamma+1)\}, \quad m \text{ even},$$

in the second one. With our approach, choosing $p=m+1$, $q=1$ in $\varphi_1(t)$ in the first case, and $p=q=m+1$ in the second one, by applying (3.1) with $j=l=0$, from the Theorem 2 above, for example, we obtain the error estimates

$$O(n^{-2(m+1)(\sigma+1)}) \tag{3.6}$$

and

$$O(n^{-2(m+1)(\delta+1)}), \tag{3.7}$$

where $\delta=\min\{\sigma,\gamma\}$, respectively.

From Tables 5–10, we have compared the absolute errors produced by our approach, based on the transformation $\varphi_1(t)$ and the n-point Gauss–Legendre rule, with those generated by the n-point Trapezoidal rule. The Trapezoidal rule was applied after introducing a change of variable using a symmetric form of $\varphi_3(t)$, with exponents $p=q$ equal to the maximum one in $\varphi_1(t)$.

In the case of the Trapezoidal rule we have used the rational transformation $\varphi_3(t)$, since in all examples we have considered it has given slightly better results.

Table 6
Absolute errors obtained by Gauss–Legendre (with φ_1) and Trapezoidal (with φ_3) rules when $f(x)=x\log x$

	p	q	$n=2$	$n=4$	$n=8$	$n=16$	$n=32$	$n=64$	$n=128$
φ_1	2	1	1.23E−02	3.15E−05	1.46E−07	6.70E−10	2.90E−12	1.19E−14	—
and	3	1	7.89E−02	1.42E−05	2.50E−09	6.85E−13	—	—	—
G.L.	4	1	1.11E−01	9.60E−05	1.70E−10	—	—	—	—
	5	1	1.00E−01	2.96E−03	3.96E−11	—	—	—	—
φ_3	2	2	9.81E−03	1.04E−04	1.87E−05	1.68E−06	1.34E−07	1.01E−08	7.27E−10
and	3	3	9.50E−02	8.53E−03	2.32E−05	5.40E−09	1.16E−10	2.27E−12	4.20E−14
T.	4	4	1.76E−01	4.39E−02	9.28E−04	1.15E−07	1.83E−13	—	—
	5	5	2.20E−01	9.59E−02	6.22E−03	7.36E−06	2.52E−12	—	—

Table 7
Absolute errors obtained by Gauss–Legendre (with φ_1) and Trapezoidal (with φ_3) rules when $f(x)=2\log x+\log(1-x)$

	p	q	$n=2$	$n=4$	$n=8$	$n=16$	$n=32$	$n=64$	$n=128$
φ_1	2	2	4.26E−01	2.52E−02	1.79E−03	1.23E−04	8.12E−06	5.23E−07	3.32E−08
and	3	3	4.66E−01	1.76E−02	2.69E−04	4.58E−06	7.65E−08	1.24E−09	1.98E−11
G.L.	4	4	1.63E−01	5.48E−02	7.71E−05	2.96E−07	1.23E−09	5.06E−12	2.80E−14
	5	5	2.82E−01	1.70E−01	4.50E−05	3.03E−08	3.07E−11	3.55E−14	1.11E−14
φ_3	2	2	3.61E−01	1.51E−01	5.30E−02	1.69E−02	5.06E−03	1.46E−03	4.12E−04
and	3	3	8.67E−02	9.02E−03	7.15E−04	1.31E−04	1.99E−05	2.76E−06	3.66E−07
T.	4	4	1.16E−01	5.34E−02	1.46E−03	1.78E−05	1.44E−06	1.10E−07	8.00E−09
	5	5	6.68E−01	5.04E−02	8.62E−03	8.94E−06	1.03E−08	4.16E−10	1.49E−11

Table 8
Absolute errors obtained by Gauss–Legendre (with φ_1) and Trapezoidal (with φ_3) rules when $f(x) = 2x\log x + (1-x)\log(1-x)$

	p	q	$n=2$	$n=4$	$n=8$	$n=16$	$n=32$	$n=64$	$n=128$
φ_1	2	2	2.14E−01	1.29E−03	4.41E−06	1.86E−08	7.89E−11	3.25E−13	—
and	3	3	4.43E−01	2.10E−02	1.43E−06	2.35E−10	5.77E−14	—	—
G.L.	4	4	5.86E−01	7.92E−02	2.03E−06	1.26E−11	—	—	—
	5	5	6.66E−01	1.54E−01	9.21E−05	3.70E−12	—	—	—
φ_3	2	2	2.94E−02	3.11E−04	5.62E−05	5.03E−06	4.02E−07	3.02E−08	2.18E−09
and	3	3	2.85E−01	2.56E−02	6.97E−05	1.62E−08	3.48E−10	6.80E−12	1.26E−13
T.	4	4	5.27E−01	1.32E−01	2.78E−03	3.46E−07	5.49E−13	—	—
	5	5	6.60E−01	2.88E−01	1.87E−02	2.21E−05	7.55E−12	—	—

Table 9
Absolute errors obtained by Gauss–Legendre (with φ_1) and Trapezoidal (with φ_3) rules when $f(x)=x^{1/5}$

	p	q	$n=2$	$n=4$	$n=8$	$n=16$	$n=32$	$n=64$	$n=128$
φ_1	2	1	2.62E−03	1.23E−04	5.42E−06	2.20E−07	8.47E−09	3.15E−10	1.15E−11
and	3	1	2.17E−02	1.35E−05	1.12E−07	8.90E−10	6.66E−12	4.86E−14	—
G.L.	4	1	1.65E−02	2.29E−06	3.10E−09	4.69E−12	—	—	—
	5	1	6.94E−02	—	—	—	—	—	—
φ_3	2	2	2.64E−02	7.73E−03	2.36E−03	6.48E−04	1.68E−04	4.24E−05	1.06E−05
and	3	3	1.13E−01	5.39E−03	1.80E−05	2.28E−06	1.81E−07	1.38E−08	1.05E−09
T.	4	4	3.17E−01	4.45E−02	4.88E−04	3.59E−07	2.81E−08	1.87E−09	1.21E−10
	5	5	5.05E−01	1.29E−01	4.41E−03	2.68E−06	1.07E−10	1.84E−12	3.01E−14

Table 10
Absolute errors obtained by Gauss–Legendre (with φ_1) and Trapezoidal (with φ_3) rules when $f(x)=x^{-1/5}$

	p	q	$n=2$	$n=4$	$n=8$	$n=16$	$n=32$	$n=64$	$n=128$
φ_1	2	1	1.08E−02	1.52E−03	1.94E−04	2.31E−05	2.63E−06	2.93E−07	3.23E−08
and	3	1	3.93E−03	1.84E−04	8.13E−06	3.31E−07	1.27E−08	4.73E−10	1.73E−11
G.L.	4	1	1.78E−03	2.34E−05	3.43E−07	4.71E−09	6.09E−11	7.57E−13	1.22E−14
	5	1	—	—	—	—	—	—	—
φ_3	2	2	8.58E−02	3.44E−02	1.27E−02	4.39E−03	1.46E−03	4.80E−04	1.57E−04
and	3	3	1.05E−01	5.63E−03	4.57E−04	1.06E−04	2.23E−05	4.45E−06	8.66E−07
T.	4	4	3.28E−01	3.75E−02	2.98E−04	3.39E−06	3.46E−07	3.55E−08	3.72E−09
	5	5	5.85E−01	1.22E−01	3.29E−03	1.07E−06	3.48E−08	2.33E−09	1.50E−10

Our approach has been implemented using the Gauss–Legendre rule, instead of the more natural Gauss–Radau or Gauss–Lobatto formula, because in general it has shown to be slightly more efficient.

The use of an extrapolation technique improves the results given by the Trapezoidal rule; however, even these are much less accurate than those obtained with our approach.

4. Integration over a triangle

In this section we consider integrals over the reference triangle $0\leqslant x\leqslant 1$, $0\leqslant y\leqslant x$, of functions which may have a (weak) full corner singularity (see [15]) of the form

$$I=\int_0^1\int_0^x w(x,y)g(x,y)\,\mathrm{d}y\,\mathrm{d}x \tag{4.1}$$

with

$$w(x,y)=y^{\lambda}(x-y)^{\mu}(1-x)^{\nu}r^{\beta}\log^k r,\quad r=\sqrt{x^2+ay^2},\quad k=0,1,$$

where we assume λ, μ, $\nu>-1$, $\mu+\lambda+\beta>-2$, $a>0$ a real constant, and $g(x,y)$ smooth. In general, one has to deal with integrals which refer to a general triangle; however, by means of an affine transformation these integrals can always be reduced to the corresponding ones of the form (4.1).

Integrals of this type arise, for example, in the numerical solution of boundary integral equations over polyhedral boundaries by Galerkin BEM's. They have been considered in [15,16], where extrapolation techniques have been proposed and examined.

In [15] it was noted that methods which apply a cubature rule with a (fixed) weight function (containing a singular part) would not be appropriate, since a transformation to take the integral to a reference triangle would change the weight function. This problem is alleviated by the approach we suggest, which is the natural extension of the one we have proposed in the previous section.

Before applying the smoothing transformation, we introduce the change of variable $y = ux$ in (4.1); we obtain

$$I = \int_0^1 x^{\mu+\beta+\lambda+1}(1-x)^{\nu} \int_0^1 u^{\lambda}(1-u)^{\mu}(1+au^2)^{\beta/2}[\log(x\sqrt{1+au^2})]^k \; g(x,ux)\,\mathrm{d}u\,\mathrm{d}x.$$

Notice that in the case $k = 1$, for example, we can further write

$$\begin{aligned} I &= \int_0^1 x^{\mu+\beta+\lambda+1}(1-x)^{\nu} \log x \int_0^1 u^{\lambda}(1-u)^{\mu}(1+au^2)^{\beta/2} \; g(x,ux)\,\mathrm{d}u\,\mathrm{d}x \\ &\quad + \frac{1}{2}\int_0^1 x^{\mu+\beta+\lambda+1}(1-x)^{\nu} \int_0^1 u^{\lambda}(1-u)^{\mu}(1+au^2)^{\beta/2}\log(1+au^2) \; g(x,ux)\,\mathrm{d}u\,\mathrm{d}x \\ &:= I_1 + I_2. \end{aligned} \tag{4.2}$$

The above change of variable is often called Duffy's transformation (see [7]), but it has been already used a few years earlier in [10]. It eliminates the corner singularity, leaving only the singularities along the edges of the unit square.

Since I_1 and I_2 in (4.2) are very similar, we will consider only one of them, namely I_1. To compute it, we propose first to introduce smoothing changes of variable $x = \varphi_1(t)$, $u = \bar{\varphi}_1(s)$, where φ_1 and $\bar{\varphi}_1$ are both of type φ_1, but in general with different smoothing exponents depending on $\mu+\beta+\lambda$, ν, λ and μ. Then we approximate each one-dimensional integral by the n-point Gauss–Legendre rule. We obtain the following product formula:

$$I_1 = \int_0^1 F(t)\int_0^1 G(t,s)\,\mathrm{d}s\,\mathrm{d}t = \sum_{i=1}^{n} w_{ni}F(t_{ni})\sum_{j=1}^{n} w_{nj}G(t_{ni},t_{nj}) + R_n,$$

where we have set

$$F(t) = [\varphi_1(t)]^{\mu+\beta+\lambda+1}[1-\varphi_1(t)]^{\nu}\log\varphi_1(t)\;\varphi_1'(t)$$
$$G(t,s) = [\bar{\varphi}_1(s)]^{\lambda}[1-\bar{\varphi}_1(s)]^{\mu}[1+a\bar{\varphi}_1(s)^2]^{\beta/2}g(\varphi_1(t),\varphi_1(t)\bar{\varphi}_1(s))\;\bar{\varphi}_1'(s).$$

Of course, in general, one could use a n-point Gauss–Legendre rule for the inner integral, and a m-point rule for the outer integral with $n \neq m$.

To examine the behaviour of the remainder term R_n we need to recall an extension of the convergence results presented in Section 2, recently obtained in [19]. In particular, it has been shown in [19] how these results can be extended to include functions $f(x)$ like those in Theorems 1–4

Table 11
Absolute errors obtained for $\lambda \equiv \mu \equiv \nu = \frac{1}{2}$, $\beta = 1$, $k = 1$ and $g(x,y) = e^{x+y}$

p	q	$n = 2$	$n = 4$	$n = 8$	$n = 16$	$n = 32$	$n = 64$
2	2	8.93E−02	1.58E−02	2.11E−05	—	—	—
3	3	9.64E−02	5.34E−03	1.42E−04	1.79E−09	2.61E−12	—
4	4	5.98E−02	2.52E−02	2.63E−03	2.16E−08	—	—
5	5	3.23E−02	5.68E−02	6.94E−03	1.50E−06	—	—

Table 12
Absolute errors obtained for $\lambda \equiv \mu \equiv \nu = \frac{1}{5}$, $\beta = 1$, $k = 1$ and $g(x,y) = 1$

p	q	$n = 2$	$n = 4$	$n = 8$	$n = 16$	$n = 32$	$n = 64$
2	2	7.12E−02	7.54E−03	1.16E−05	4.65E−07	1.78E−08	6.62E−10
3	3	9.25E−02	9.66E−03	1.66E−04	8.20E−09	5.98E−11	4.25E−13
4	4	7.30E−02	2.06E−02	1.24E−03	8.29E−10	2.77E−13	—
5	5	5.05E−02	4.48E−02	3.10E−03	6.55E−08	—	—

multiplied by an extra term $g(x,y)$ (smooth with respect to both variables x and y, $0 \leqslant y \leqslant 1$). With these new results it is not difficult to derive the following bound:

$$|R_n| = O(n^{-2p(\mu+\beta+\lambda+2)} \log n) + O(n^{-2q(\nu+1)} \log n) + O(n^{-2\bar{p}(\lambda+1)}) + O(n^{-2\bar{q}(\mu+1)}),$$

where p, q are the smoothing exponents of $\varphi_1(t)$, while $\bar{p}$, $\bar{q}$ are the smoothing exponents of $\bar{\varphi}_1(s)$.

In Tables 11–12 we report some results obtained by applying our approach.

All computations have been performed on a PC using 16-digit double precision arithmetic. Nodes and weights of the Gauss rules have been determined with 14 significant digits.

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