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Variable Order Composite Quadrature of Singular and Nearly Singular Integrals*

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Abstract — Zusammenfassung

Variable Order Composite Quadrature of Singular and Nearly Singular Integrals. A class of variable order composite quadrature formulas for the numerical integration of functions with a singularity in or near to the region of integration is introduced. Exponential convergence of the method is shown for all integrands in the countably normed space $\mathscr{B}_\beta$. Numerical examples are presented which demonstrate that the asymptotic exponential convergence rates obtained here are sharp and already observed for a small number of quadrature points.

AMS Subject Classification: Primary: 65D30, 41A55; Secondary: 65D32

Key words: Singular integrals, numerical integration, exponential convergence.

Zusammengesetzte Quadratur variabler Ordnung für singuläre und fastsinguläre Integrale. Wir stellen eine Klasse von zusammengesetzten Quadraturformeln variabler Ordnung vor, die sich zur numerischen Integration von Funktionen mit einer Singularität im Inneren oder in der Nähe des Integrationsbereichs eignen. Für alle Integranden in dem abzählbar normierten Raum $\mathscr{B}_\beta$ wird eine exponentielle Konvergenz des Verfahrens bewiesen. Numerische Beispiele zeigen, daß die ermittelten asymptotischen exponentiellen Konvergenzraten scharf sind und schon bei einer kleinen Zahl von Quadraturknoten erreicht werden.

1. Introduction

In recent years, the numerical quadrature of functions with radial singularities in or near to the (two or three dimensional) domain of integration has received much attention, primarily due to the increasing use of techniques based on integral equations, such as, for example, the boundary element method (BEM) and vortex methods, for the solution of complex engineering problems (see, for example, [6, 7] and [12] and the references there). In the BEM singular and nearly singular integrals arise as diagonal, respectively sub- and superdiagonal elements in the stiffness matrices of the discretized boundary integral operators. They also arise when the representation formula is evaluated at a point near to, or on the boundary surface. Since the integrations are often in local coordinates on curved surfaces in $\mathbb{R}^3$, the

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integrands $f(x)$ do *not* behave like

$$f(x) = |x|^\alpha g(x)$$

in the local coordinates $x = (x_1, x_2)$ parametrizing the surface where $|x|^2 = x_1^2 + x_2^2$ and $g(x)$ is a smooth (analytic) function. This precludes the use of weighted quadratures, but owing to the general structure of the underlying boundary integral operators [13], the integrands have yet enough properties to be treated efficiently with several methods (for example, polar coordinates and modified extrapolation, see [12]).

In the case of *nearly singular* integrals, however, the additional problem arises that the location of the singular point (for example, a collocation or nodal point in an adjacent boundary element) in the local coordinates of integration is not explicitly known. What is usually known (or can be computed with reasonable effort) is the point closest to the singular point in the domain of integration.

Therefore a quadrature scheme is required that can provide highly accurate numerical integration based solely on this information, *uniformly* for integrand classes which contain both singular and nearly singular functions alike.

Two broad groups of techniques for the numerical evaluation of singular and nearly singular integrals can be distinguished: semi-analytical and purely numerical techniques. In the former, the integrands are subject to certain analytic transformations (regularizing coordinate transformation, separation into a singular and regular part etc.) prior to numerical integration (see, e.g., [6–8]) while in the latter, special numerical quadrature techniques, such as weighted quadratures, modified extrapolation (see, e.g., [9]) can be found.

A particular purely numerical technique for integrands with point singularities has been recently introduced by Yang and Atkinson [15]. They subdivide the region of integration nonuniformly with the size of the subdomains decreasing towards the singular point and apply a properly scaled quadrature rule on each subdomain. They prove that in this fashion a rate of convergence of $O(N^{-2})$ can be achieved independently of the strength of the singularity (here and throughout this paper, N denotes the number of integrand evaluations). This result is closely related to the fact that functions with a radial singularity can be optimally approximated by piecewise polynomials on a properly graded mesh.

The approach introduced in the present paper corresponds to what is known in FE analysis as $h-p$ version [4], where strongly refined, geometric meshes are combined with different polynomial degrees—here we combine elementary quadrature formulae of varying orders in subdomains the size of which decreases geometrically towards the singular point. We prove that this yields *exponential convergence* of order

$$O(\exp(-bN^{1/(r+1)})) \tag{1.1}$$

for integrands in the countably normed space $\mathscr{B}_\beta$ where $b > 0$ is a constant and r is the dimension of the region of integration (typically, $r = 1, 2, 3$). The scheme has two parameters, the geometric grading factor $\sigma \in (0, 1)$ and the slope of the degree vector μ, which can be used to optimize the constants in the estimate (1.1) for a given application. In addition, our convergence proof is sufficiently flexible and the class $\mathscr{B}_\beta$ sufficiently large in order to handle multiple singularities, mapped domains of integration and also a wide variety of elementary cubature formulae used to construct the composite rule leaving room for further optimization of the method. In numerical experiments we show that the convergence estimate (1.1) is sharp and that, as a rule, $\mu \sim 1$ and $0.1 < \sigma < 0.2$ are optimal. The geometrically graded subdivisions of the domain of integration thus obtained deviate substantially from those generated by adaptive integrators which use selective bisection of subdomains (corresponding to $\sigma = 0.5$). We also demonstrate numerically the robustness of the method for nearly singular integrals where the distance of the singular point versus the diameter of the integration domain varies from 1 to 10^{-6}. As to the limitations of the method, we show in [14] that for nearly singular potential integrals which jump as the source point passes through the surface (as, for example, the double layer in classical potential theory), a robust and efficient numerical method must incorporate the analytical jump relations of the potential. For such integrands (which do not belong uniformly to $\mathscr{B}_\beta(\Omega)$), we show with a numerical example that the accuracy of the variable order, composite quadratures introduced here deteriorates slowly as the source point approaches the domain of integration.

The outline of this paper is as follows: in Section 2 we define notation and the spaces used, in particular weighted Sobolev spaces of fractional order and the countably normed spaces $\mathscr{B}_\beta$. Some important examples of integrands belonging to $\mathscr{B}_\beta$ are also exhibited. In Section 3 we describe the variable order, composite quadratures in the special setting of a unit square in $\mathbb{R}^2$ with the singular point O located in the origin. In Section 4 we prove for this case the exponential convergence (1.1) of the method for arbitrary integrands $f \in \mathscr{B}_\beta$. Section 5 discusses several generalizations of the convergence result to other domains, multiple singularities, and dimensions other than 2. Section 6 is devoted to numerical examples which show in particular the exponential convergence estimate (1.1) to be sharp.

2. Preliminaries

2.1 Notation

By $\mathbb{R}^r$ we denote the r dimensional Euclidean space of points $x = (x_1, \dots, x_r)$, by $K = (0,1)^r$ the (open) unit cube in $\mathbb{R}^r$ and by $T = \{x \in \mathbb{R}^r | x_i > 0,\ x_1 + \cdots + x_r < 1\}$ the unit simplex. The Euclidean distance of x to the origin O is $\rho = |x| = (x_1^2 + \cdots + x_r^2)^{1/2}$. The closure of an open, nonempty set $\Omega \subset \mathbb{R}^r$ is denoted by $\overline{\Omega}$, its boundary $\overline{\Omega} \backslash \Omega$ by $\partial\Omega$ and its volume by $|\Omega|$.

2.2 *Sobolev Spaces*

For every open, polyhedral domain $\Omega \subset \mathbb{R}^r$ we denote by $L^p(\Omega)$, $1 \leq p < \infty$ the usual spaces of functions f for which $|f|^p$ is integrable. Further, for every nonnegative integer m we denote by $H^m(\Omega)$ the Sobolev space of functions with generalized derivatives of order not exceeding m in $L^2(\Omega)$ furnished with the norm

$$\|f\|^2_{H^m(\Omega)} = \sum_{0 \leq k \leq m} \|D^k f\|^2_{L^2(\Omega)}, \qquad \|D^k f\|^2_{L^2(\Omega)} = \sum_{|\alpha| = k} \|D^\alpha f\|^2_{L^2(\Omega)}$$

where $\alpha \in \mathbb{N}_0^2$ is a multiindex, $|\alpha| = \alpha_1 + \alpha_2 + \cdots + \alpha_r$, and, as usual

$$D^\alpha f = \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha_1} \ldots \partial x_r^{\alpha_r}}.$$

We will also write

$$|D^m f|^2 = \sum_{|\alpha| = m} |D^\alpha f|^2.$$

2.3 *The spaces $\mathscr{B}_\beta(\Omega)$*

For a parameter $0 < \beta < r/2$ and $\Omega = K, T$ we denote by $H^m_\beta(\Omega)$ the closure of $C^\infty(\bar{\Omega})$ with respect to the weighted norm

$$\|f\|^2_{H^m_\beta(\Omega)} = \sum_{k=0}^{m} |f|^2_{H^k_\beta(\Omega)}, \qquad |f|^2_{H^k_\beta(\Omega)} = \int_\Omega |D^k f|^2 \Phi^2_{\beta+k}(x)\, dx \tag{2.1}$$

where, for $t \in \mathbb{R}$, the weight is given by $\Phi_t(x) = |x|^t$.

The spaces $\mathscr{B}_\beta(\Omega)$ consist of functions that are analytic in Ω, but possibly singular at the origin O. Functions in $\mathscr{B}_\beta(\Omega)$ will be characterized by the growth of their derivatives, i.e. we require that

$$\left(\int_\Omega |D^\alpha f|^2 \Phi^2_{\beta+k}(x)\, dx \right)^{1/2} \leq C_f (d_f)^k k! \qquad \forall |\alpha| = k \in \mathbb{N}_0 \tag{2.2}$$

holds with constants $C_f > 0$ and $d_f \geq 1$ which depend only on f, but not on k. Then we define

$$\mathscr{B}_\beta(\Omega) = \{ f \mid f \in L^1(\Omega) \cap H^m_\beta(\Omega)\ \forall m \in \mathbb{N}_0, (2.2) \text{ holds} \}. \tag{2.3}$$

These spaces are countably normed spaces [5] and were first introduced in the analysis of the $h-p$ finite element method in [4]. Functions in $\mathscr{B}_\beta(\Omega)$ are characterized by the best constants C_f and d_f in (2.2). If $O \notin \bar{\Omega}$, functions in $\mathscr{B}_\beta(\Omega)$ are analytic in $\bar{\Omega}$.

2.4 *Fractional Order Spaces*

For $s \in \mathbb{R}^+ \backslash \mathbb{N}$, $H^s_\beta(\Omega)$ is defined as interpolation space. More precisely, since $H^{k+1}_\beta(\Omega) \subset H^k_\beta(\Omega)$, we may define $H^{k+\theta}_\beta(\Omega)$ for $0 < \theta < 1$ via the K-method of interpolation [1]:

$$H_\beta^{k+\theta}(\Omega) = (H_\beta^k(\Omega), H_\beta^{k+1}(\Omega))_{\theta,\infty} \qquad \forall k \in \mathbb{N}_0, \qquad 0 < \theta < 1.$$

From the interpolation inequality

$$\|f\|_{H_\beta^{k+\theta}(\Omega)} \leq \|f\|_{H_\beta^k(\Omega)}^{1-\theta} \|f\|_{H_\beta^{k+1}(\Omega)}^{\theta} \tag{2.4}$$

we find for $f \in \mathscr{B}_\beta(\Omega)$ that

$$\|f\|_{H_\beta^{k+\theta}(\Omega)} \leq C_f d_f^{k+\theta}(k+\theta)^{1/2}\Gamma(k+1+\theta) \qquad \forall k \in \mathbb{N}_0, \qquad 0 < \theta < 1. \tag{2.5}$$

2.5 Examples of $u \in \mathscr{B}_\beta(\Omega)$

2.5.1. Consider $\Omega = K = (0,1)$ and the model family of almost singular integrands

$$f_\varepsilon(x) = (x+\varepsilon)^\lambda, \qquad \varepsilon \geq 0, \qquad -1 < \lambda < 0. \tag{2.6}$$

Then we have

Proposition 2.1. *For $\beta > -1/2 - \lambda$, $f_\varepsilon(x) \in \mathscr{B}_\beta(K)$ for every $\varepsilon \geq 0$ and* (2.2) *holds with $d_f = 2$ and with $C_f = (2(\beta+\lambda)+1)^{-1/2}$.*

Proof: We verify condition (2.2). Since for $k \in \mathbb{N}$

$$f^{(k)}(x) = \lambda(\lambda-1)\dots(\lambda-k+1)(x+\varepsilon)^{\lambda-k},$$

we find

$$\begin{aligned}|f^{(k)}(x)\Phi_{\beta+k}(x)| &\leq (k-\lambda)(k-1-\lambda)\dots(1-\lambda)\lambda|x+\varepsilon|^{\lambda-k}|x|^{\beta+k}\\ &\leq (k+1)!\,|x|^\beta|x+\varepsilon|^\lambda\end{aligned}$$

where we used that $|x| \leq |x+\varepsilon|$ for $0 \leq x \leq 1$ and every $\varepsilon \geq 0$. Hence

$$\int_K |D^k f|^2 \Phi_{\beta+k}^2(x)\,dx \leq (k+1)^2(k!)^2 \int_0^1 x^{2(\lambda+\beta)}\,dx \leq \frac{1}{2(\lambda+\beta)+1} 2^{2k}(k!)^2$$

from where the assertion follows. □

2.5.2. Consider $\Omega = K = (0,1)^2$ and the family

$$f_\varepsilon(\rho) = (\varepsilon+\rho)^\lambda \qquad \varepsilon \geq 0, \qquad -2 < \lambda < 0. \tag{2.7}$$

Then we have

Proposition 2.2. *For $\beta > -1 - \lambda$, $f_\varepsilon(\rho) \in \mathscr{B}_\beta(K)$ uniformly for $0 \leq \varepsilon \leq 1$.*

The proof of this proposition is elementary, but lengthy and therefore presented in the Appendix.

The crucial point with both of these examples is that the one-parameter families f_ε belong *uniformly* to $\mathscr{B}_\beta$ (i.e. the constants C_f and d_f in (2.2) are independent of ε). Therefore a quadrature strategy which performs on the class $\mathscr{B}_\beta$ will integrate $f_\varepsilon(x)$ *regardless of the particular value of* ε, i.e. the explicit location of the singularity is not needed.

3. A Class of Variable Order Composite Quadratures

Our purpose is the numerical evaluation of

$$If = \int_\Omega f(x)\,dx$$

where $\Omega = K$ or $\Omega = T$ and $f \in \mathscr{B}_\beta(\Omega)$. We will present the construction and the analysis of the composite quadrature formulas in detail for the case $\Omega = K \subset \mathbb{R}^2$ and $O = (0,0)$ and elaborate on $\Omega = T$ in Section 5 below. To construct the composite formulas, we partition K into a collection K_σ^n of smaller squares where $b \in \mathbb{N}$ and $0 < \sigma < 1$. To this end, we define

$$x_1^0 = x_2^0 = 0, \qquad x_1^j = x_2^j = \sigma^{n+1-j}, \qquad 1 \le j \le n+1, \qquad 0 < \sigma < 1, \quad (3.1)$$

$$\begin{aligned} K_{1,j} &= (x_1^{j-1}, x_1^j) \times (0, x_2^{j-1}) && \text{for } 2 \le j \le n+1, \\ K_{2,j} &= (x_1^{j-1}, x_1^j) \times (x_2^{j-1}, x_2^j) && \text{for } 1 \le j \le n+1, \\ K_{3,j} &= (0, x_1^{j-1}) \times (x_2^{j-1}, x_2^j) && \text{for } 2 \le j \le n+1 \end{aligned} \quad (3.2)$$

and refer to Fig. 1 for an example with $n = 3$ and $\sigma = 0.5$.

A quadrature rule $Qf = \sum_j w_j f(x_{1j}, x_{2j})$ on K is of type PI, if its weights w_j are positive and $(x_{1j}, x_{2j}) \in \bar{K}$. It is a rule of *total degree p* denoted by Q^p, if it is exact

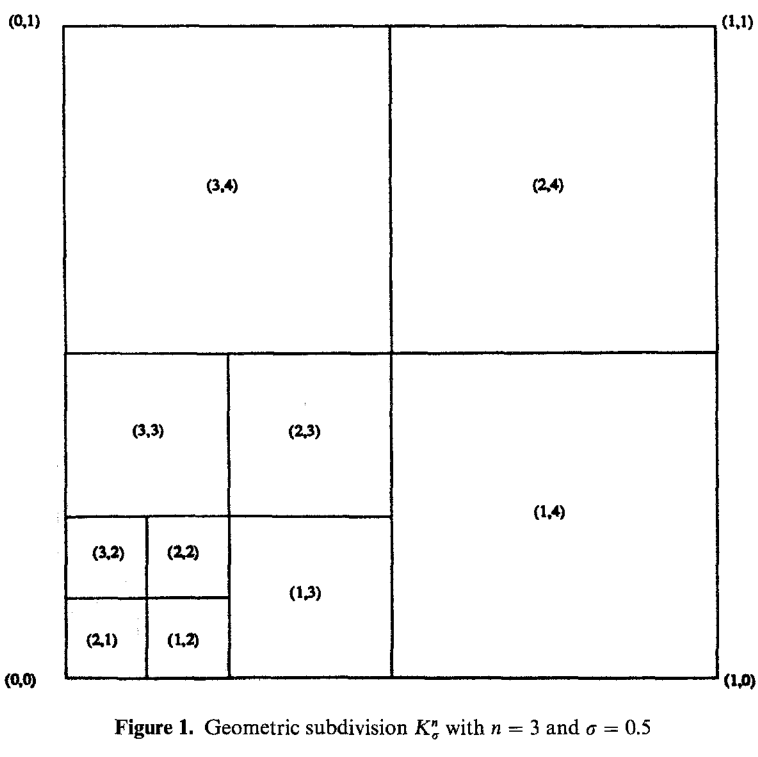

Figure 1. Geometric subdivision K_σ^n with $n = 3$ and $\sigma = 0.5$

for polynomial integrands of total degree p, i.e. the quadrature error Ef satisfies

$$Ef := If - Q^p f = 0 \qquad \forall f = \sum_{0 \le i,j \le p} c_{ij} x_1^i x_2^i . \tag{3.3}$$

Let a family $\mathcal{Q} = \{Q^p\}_{p=0}^{\infty}$ of PI rules of total degree p on K be given. For a given $n \in \mathbb{N}$ we associate with the subdomains $K_{i,j} \in K_\sigma^n$, $i = 1,2,3$, polynomial degrees p_j which we collect in the *degree vector* $\mathbf{p}$ and define the composite quadrature rule $Q_\sigma^{n,\mathbf{p}}$ by composing properly scaled copies $Q_{i,j}^{p_j}$ of $Q^{p_j} \in \mathcal{Q}$ on $K_{i,j}$ of total degree p_j for $j \ge 2$, i.e.

$$Q_\sigma^{n,\mathbf{p}} f = \sum_{j=2}^{n+1} \sum_{i=1}^{3} Q_{i,j}^{p_j} f. \tag{3.4}$$

Remark 3.1. Note that we ignore in (3.4) the contribution from $K_{1,1}$ so that $Q_\sigma^{n,\mathbf{p}} f$ is well defined even if the component rules Q^{p_i} require function values at the origin.

4. Analysis of the Quadrature Error

In this section we prove that the composite quadratures (3.4) converge exponentially with respect to the number N of integrand evaluations for any $f \in \mathcal{B}_\beta(K)$.

Theorem 4.1. *Let $f \in \mathcal{B}_\beta(K)$ for some $0 < \beta < 1$. Then, for every $0 < \sigma < 1$ and a linear degree vector* $\mathbf{p}$

$$p_j = \max\{2, \lfloor j\mu \rfloor + 1\} \qquad 2 \le j \le n+1 \tag{4.1}$$

with slope

$$\mu > \frac{(1-\beta)\ln \sigma}{\ln F_{min}} \tag{4.2}$$

and F_{min} defined in (4.13) *below, there exists a constant $b > 0$ independent of N such that*

$$\left| \int_K f(x)\,dx - Q_\sigma^{n,\mathbf{p}} f \right| \le C C_f \exp(-bN^{1/3}) \tag{4.3}$$

where C depends on σ, β, μ, d_f and C_f and d_f are the constants in (2.2).

For the proof of Theorem 4.1 we need several Lemmas. We begin with a classical estimate which relates the quadrature error to the pointwise best approximation of the integrand by polynomials.

Lemma 4.1. *Let $f \in C^0(\overline{\Omega})$, $\Omega \subset \mathbb{R}^r$, and let Q be a PI quadrature rule on Ω which is exact of total degree $p \ge 0$. Then*

$$\left| \int_\Omega f\,dx - Qf \right| \le 2|\Omega| \inf_\pi \| f - \pi \|_{L^\infty(\Omega)} \tag{4.4}$$

where the infimum is taken over all polynomials π of total degree p.

Proof: Define the error functional

$$Ef = \int_\Omega f\,dx - Qf$$

and observe that $E\pi = 0$ for all polynomials π of total degree p. Since Q is PI

$$|Ef| = |E(f-\pi)| \le \int_\Omega |f-\pi|\,dx + \sum_i w_i |(f-\pi)(x_i)|$$
$$\le \left(|\Omega| + \sum_i w_i\right) \|f-\pi\|_{L^\infty(\Omega)}.$$

Since Q is in particular exact for constants, $\sum w_i = |\Omega|$ and since π is arbitrary, the assertion follows. □

The preceding lemma shows that the quadrature error can be controlled by the pointwise best approximation of the integrand. For our estimate of the quadrature error, we require a result on the approximation of a sufficiently smooth function by polynomials from [4, Lemma 4.3].

Proposition 4.1. *Let $\Omega = (a,b) \times (c,d)$ with $h = b-a = d-c$. For every $\psi \in H^{k+3}(\Omega)$ there exists a polynomial π of total degree k such that for every integer s satisfying $1 \le s \le k$ and $0 \le m \le 2$*

$$\|D^m(\psi-\pi)\|^2_{L^2(\Omega)} \le Ch^{-2m}\frac{(k-s)!}{(k+s+2-2m)!}\left(\frac{h}{2}\right)^{2(s+1)} \cdot \sum_{l=0}^{2}\left(\frac{h}{2}\right)^{2l}\left\{\left\|\frac{\partial^{s+1+l}\psi}{\partial x_1^{s+1}\partial x_2^l}\right\|^2_{L^2(\Omega)} + \left\|\frac{\partial^{s+1+l}\psi}{\partial x_1^l\partial x_2^{s+1}}\right\|^2_{L^2(\Omega)}\right\}. \tag{4.5}$$

Here the constant C is independent of h, k and s.

Lemma 4.2. *Let $\Omega \subset K$ be as in Proposition 4.1 and $0 < \rho_0 = \operatorname{dist}(O,\Omega)$. Then for every $\psi \in H^{k+3}_\beta(K)$ there exists a polynomial π of total degree k such that for $0 \le m \le 2$ and any s with $1 \le s \le k$*

$$\|D^m(\psi-\pi)\|^2_{L^2(\Omega)} \le C\rho_0^{-2(m+\beta)}\left(\frac{\Lambda}{2}\right)^{2(s+1)}\frac{\Gamma(k-s+1)}{\Gamma(k+s+3-2m)}\|\psi\|^2_{H^{k+3}_\beta(K)} \tag{4.6}$$

where C is independent of s, k and ρ_0 and

$$0 < \lambda \le h/\rho_0 \le \Lambda < \infty. \tag{4.7}$$

Proof: We denote $|x|$ by ρ and observe that $\rho/\rho_0 > 1$ on Ω. Thus we get from (4.5) that for $1 \le \tilde{k} \le k$

$$\|D^m(\psi-\pi)\|^2_{L^2(\Omega)} \le Ch^{-2m}\frac{(k-\tilde{k})!}{(k+\tilde{k}+2-2m)!}\left(\frac{h}{2}\right)^{2(\tilde{k}+1)} \cdot \sum_{l=0}^{2}\left(\frac{h}{2}\right)^{2l}\rho_0^{-2(\beta+\tilde{k}+1+l)}\left\{\left\|\rho^{\beta+\tilde{k}+1+l}\frac{\partial^{s+1+l}\psi}{\partial x_1^{s+1}\partial x_2^l}\right\|^2_{L^2(\Omega)} + \left\|\rho^{\beta+\tilde{k}+1+l}\frac{\partial^{s+1+l}\psi}{\partial x_1^l\partial x_2^{s+1}}\right\|^2_{L^2(\Omega)}\right\}.$$

Due to (4.7) we estimate

$$\|D^m(\psi - \pi)\|^2_{L^2(\Omega)} \leq \frac{C}{\lambda^{2m}} \rho_0^{-2m-2\beta} \left(\frac{\Lambda}{2}\right)^{2(\tilde{k}+1)} \frac{(k-\tilde{k})!}{(k+\tilde{k}+2-2m)!} \sum_{l=0}^{2} \left(\frac{\Lambda}{2}\right)^{2l} |\psi|^2_{H_\beta^{\tilde{k}+1+l}(K)}$$

$$\leq C\rho_0^{-2m-2\beta} \left(\frac{\Lambda}{2}\right)^{2(\tilde{k}+1)} \frac{(k-\tilde{k})!}{(k+\tilde{k}+2-2m)!} \|\psi\|^2_{H_\beta^{\tilde{k}+3}(K)}$$

where the constant C depends on λ, Λ, but is independent of k, $\tilde{k}$ and ρ_0.

Next, consider the operator $T\psi = D^m(\psi - \pi)$. Then T: $H_\beta^{\tilde{k}+3}(K) \to L^2(\Omega)$ continuously and

$$\|T\|^2_{H_\beta^{\tilde{k}+3}(K) \to L^2(\Omega)} \leq C\rho_0^{-2(m+\beta)} \left(\frac{\Lambda}{2}\right)^{2(\tilde{k}+1)} \frac{(j-\tilde{k})!}{(k+\tilde{k}+2-2m)!}.$$

For $0 < \theta < 1$ define $s = \tilde{k} - 1 + \theta$ and recall that

$$H_\beta^{s+3}(K) = (H_\beta^{k+2}(K), H_\beta^{k+3}(K))_{\theta,\infty}.$$

Then T: $H_\beta^{s+3}(K) \to L^2(\Omega)$ continuously and we find with (2.4) that

$$\|T\|^2_{H_\beta^{s+3}(K) \to L^2(\Omega)} \leq C\rho_0^{-2(m+\beta)} \left(\frac{\Lambda}{2}\right)^{2(s+1)} \frac{\Gamma(k-s+1)}{\Gamma(k+s+3-2m)}.$$

□

Remark 4.1. If $\Omega = K_{i,j} \in K_\sigma^n$ with $j \geq 2$ and $0 < \sigma < 1$, (4.7) holds with $\Lambda = (1-\sigma)/\sigma$ and $\lambda = (1-\sigma)/(\sqrt{2}\sigma)$, since it follows from (3.2) that

$$\rho_0 = \operatorname{dist}(O, K_{i,j}) = \begin{cases} \sigma^{n+2-j} & \text{for } i = 1, 3 \\ \sqrt{2}\sigma^{n+2-j} & \text{for } i = 2 \end{cases}$$

and $h = h_j = \sigma^{n+1-j}(1-\sigma)$.

Proposition 4.1 states that a polynomial π can be found so that (4.5) holds simultaneously for $0 \leq m \leq 2$. To control the quadrature error it is thus necessary to estimate $\|\varphi\|_{L^\infty(\Omega)}$ in terms of $|\varphi|_{H^m(\Omega)}$ with the Sobolev embedding theorem where care must be taken to keep the dependence of the constants on the size of the domain explicit.

Lemma 4.3. *Let* $\Omega = (-h/2, h/2)^r \subset \mathbb{R}^r$ *with* $0 < h < 1$ *and* $l > r/2$ *a natural number. Then we have for euery* $\psi \in H^l(\Omega)$

$$\|\psi\|^2_{L^\infty(\Omega)} \leq C \sum_{0 \leq m \leq l} h^{2m-r} |\psi|^2_{H^m(\Omega)} \tag{4.8}$$

where the constant C depends on r, but is independent of h.

Proof: Denote by C the open cone

$$\mathscr{C} = \{x \in \mathbb{R}^r | 0 < |x| < h/2, x/|x| \in \Sigma\}$$

where Σ is the domain cut out of the unit sphere in $\mathbb{R}^r$ by the positive ortant $\{x \in \mathbb{R}^r | x_i > 0,\ i = 1, \ldots, r\}$. For every $x \in \overline{\Omega}$ it is then possible to find a cone

$\mathscr{C}_x \subset \Omega$ with vertex at x which is congruent to $\mathscr{C}$. Consider next a cut-off function $\chi \in C_0^\infty(\mathbb{R}^r)$ such that

1. $\chi(x) = 1$ for $|x| \le 1$,
2. $\chi(x) = 0$ for $|x| \ge 2$,
3. $|D^\alpha \chi(x)| \le M \quad \forall x, |\alpha| \le l$.

Define $\chi_\varepsilon(x) := \chi(\varepsilon x)$ and, for $y \in \mathscr{C}_x \subset \Omega$, $e_h(y) := \chi_{4/h}(y - x)$. Then

$$e_h(y) = \begin{cases} 1 & \text{for } |y - x| \le h/4 \\ 0 & \text{if } |y - x| \ge h/2 \end{cases}$$

and

$$|D^\alpha e_h(y)| \le 4^{|\alpha|} M / h^{|\alpha|} \qquad \text{if } |\alpha| \le l.$$

Let $\psi \in C^\infty(\overline{\Omega})$ and $x \in \overline{\Omega}$, $y \in \mathscr{C}_x$ and set $\vec{n} = (y - x)/|y - x|$. Then

$$\psi(x) = -e_h(x + \zeta\vec{n})\psi(x + \zeta\vec{n})|_{\zeta=0}^{\zeta=h/2} = -\int_0^{h/2} \frac{\partial(e_h\psi)}{\partial\zeta}\, d\zeta.$$

Integrating by parts l times yields

$$\psi(x) = \frac{(-1)^l}{(l-1)!} \int_0^{h/2} \zeta^{l-1} \frac{\partial^l(e_h\psi)}{\partial\zeta^l}\, d\zeta.$$

Taking absolute values and integrating both sides over $y \in \Sigma$ we find

$$\begin{aligned} |\psi(x)||\Sigma| &= \frac{1}{(l-1)!} \left| \int_{y \in \mathscr{C}_x} \zeta^{l-r} \frac{\partial^l(e_h\psi)}{\partial\zeta^l}\, dy \right| \\ &\le \left\{ \int_{\mathscr{C}_x} \zeta^{2(l-r)}\, dy \right\}^{1/2} \left\{ \int_{\mathscr{C}_x} \left| \frac{\partial^l(e_h\psi)}{\partial\zeta^l} \right|^2 dy \right\}^{1/2}, \end{aligned}$$

i.e.

$$|\psi(x)||\Sigma| \le \left\{ \int_{\mathscr{C}_x} \zeta^{2(l-r)}\, dy \right\}^{1/2} \|e_h\psi\|_{H^l(\Omega)}. \tag{4.9}$$

For the first factor in the bound (4.9), we find that

$$\int_{\mathscr{C}_x} \zeta^{2(l-r)}\, dy \le B h^{2l-r}$$

since $\zeta = |x - y|$ and $2l > r$. We estimate the second factor in (4.9). Since

$$\|e_h\psi\|_{H^l(\Omega)}^2 = \sum_{0 \le |\alpha| \le l} \int_\Omega |D^\alpha(e_h\psi)|^2\, dx$$

and, from the Leibnitz rule,

$$D^\alpha(e_h\psi) = \sum_{0 \le \beta \le \alpha} a_{\alpha\beta} D^\beta e_h D^{\alpha-\beta}\psi$$

where $\beta \leq \alpha$ is understood as $\beta_i \leq \alpha_i$ for $i = 1, \dots, r$, we estimate

$$\begin{aligned}
\|e_h\psi\|^2_{H^l(\Omega)} &\leq C \sum_{0\leq|\alpha|\leq l} \sum_{0\leq\beta\leq\alpha} \int_\Omega (D^\beta e_h D^{\alpha-\beta}\psi)^2\, dx \\
&\leq C \sum_{0\leq|\alpha|\leq l} \sum_{0\leq\beta\leq\alpha} M^2 h^{-2|\beta|} \int_\Omega (D^{\alpha-\beta}\psi)^2\, dx \\
&\leq CM^2 \sum_{0\leq|\alpha|\leq l} h^{-2|\alpha|} \sum_{0\leq\gamma\leq\alpha} h^{2|\gamma|} \|D^\gamma\psi\|^2_{L^2(\Omega)} \\
&\leq CM^2 \sum_{0\leq t\leq l} h^{-2t} \sum_{0\leq|\gamma|\leq t} h^{2|\gamma|} \|D^\gamma\psi\|^2_{L^2(\Omega)} \\
&\leq CM^2 \sum_{0\leq|\gamma|\leq l} h^{2|\gamma|} \|D^\gamma\psi\|^2_{L^2(\Omega)} \sum_{|\gamma|\leq t\leq l} h^{-2t} \\
&\leq CM^2 \sum_{0\leq m\leq l} h^{2m} |\psi|^2_{H^m(\Omega)} \sum_{m\leq t\leq l} h^{-2t}.
\end{aligned}$$

Using that $0 < h \leq 1$, we find

$$\|e_h\psi\|^2_{H^l(\Omega)} \leq CM^2 \sum_{0\leq m\leq l} h^{2m-2l} |\psi|^2_{H^m(\Omega)}$$

which yields the estimate (4.8) for $\psi \in C^\infty(\bar{\Omega})$ with a constant C independent of h. A density argument completes the proof. □

To give the proof of Theorem 4.1, it remains to estimate the error corresponding to the omission of the integral over $K_{1,1}$ (see Remark 3.1). For later use we state a r-dimensional version of the estimate required in the proof of Theorem 4.1.

Lemma 4.4. *For $n, r \in \mathbb{N}$, let $K_{1,1} = (0, \sigma^n)^r$ for some $0 < \sigma < 1$ and $K = (0,1)^r$. If $f \in H^0_\beta(K)$ for some $0 < \beta < r/2$, there holds*

$$\left| \int_{K_{1,1}} f\, dx \right| \leq C(r) \frac{\sigma^{(r/2-\beta)n}}{\sqrt{r/2-\beta}} \|f\|_{H^0_\beta(K_{1,1})}. \tag{4.10}$$

Proof: We estimate (as before, Σ denotes the domain cut out of unit sphere in $\mathbb{R}^r$ by the positive ortant)

$$\begin{aligned}
\left|\int_{K_{1,1}} f\, dx\right| &\leq \int_{K_{1,1}} |f| \rho^\beta \rho^{-\beta}\, dx \leq \left(\int_{K_{1,1}} |f|^2 \rho^{2\beta}\, dx\right)^{1/2} \left(\int_{K_{1,1}} \rho^{-2\beta}\, dx\right)^{1/2} \\
&\leq \|f\|_{H^0_\beta(K_{1,1})} \left(|\Sigma| \int_0^{\sigma^n\sqrt{r}} \rho^{r-1-2\beta}\, d\rho\right)^{1/2} \\
&= C(r) \frac{\sigma^{(r/2-\beta)n}}{\sqrt{r/2-\beta}} \|f\|_{H^0_\beta(K_{1,1})}.
\end{aligned}$$ □

We turn now to the proof of Theorem 4.1.

Proof: Throughout, the generic constant C may depend on $\beta, \sigma \in (0,1)$ and on d_f, but is independent of C_f. We proceed in several steps.

step 1: From the triangle inequality

$$|E_\sigma^{n,\mathbf{p}}f| = |If - Q_\sigma^{n,\mathbf{p}}f| \le \left|\int_{K_{1,1}} f\,dx\right| + \sum_{j=2}^{n+1}\sum_{i=1}^{3}\left|\int_{K_{i,j}} f\,dx - Q_{i,j}^{p_i}f\right|.$$

Using Lemma 4.1 and Lemma 4.4 with $r = 2$, we find

$$|E_\sigma^{n,\mathbf{p}}f| \le C\frac{\sigma^{(1-\beta)n}}{\sqrt{1-\beta}}C_f + \sum_{j=2}^{n+1}\sum_{i=1}^{3}|K_{i,j}|\inf_\pi \|f-\pi\|_{L^\infty(K_{i,j})}$$

where the infima are taken over all polynomials of total degree p_j on $K_{i,j}$. Utilizing Lemmas 4.2 and 4.3, we find for $1 \le s \le k$

$$\begin{aligned}\inf_\pi \|f-\pi\|^2_{L^\infty(K_{i,j})} &\le C\sum_{m=0}^{2} h_j^{2m-2}\inf_\pi \|D^m(f-\pi)\|^2_{L^2(K_{i,j})}\\ &\le Cr_0^{-2-2\beta}\left(\frac{A}{2}\right)^{2(s+1)}\frac{\Gamma(k-s+1)}{\Gamma(k+s-1)}\|f\|^2_{H_\beta^{s+3}(K)}\end{aligned}$$

where the constant C depends on $\sigma \in (0,1)$ but is independent of s and k. Using (4.5) and

$$h_j = x_1^j - x_1^{j-1} = \sigma^{n+1-j}(1-\sigma) = x_1^j(1-\sigma)$$

we find that

$$\inf_\pi \|f-\pi\|^2_{L^\infty(K_{i,j})} \le C(x_1^j)^{-2-2\beta}\left(\frac{A}{2}\right)^{2(s+1)}\frac{\Gamma(k-s+1)}{\Gamma(k+s-1)}\|f\|^2_{H_\beta^{s+3}(K)}.$$

step 2: Since $f \in \mathscr{B}_\beta(K)$, we have with (2.5) that

$$\begin{aligned}\inf_\pi \|f-\pi\|^2_{L^\infty(K_{i,j})} &\le C(x_1^j)^{-2-2\beta}\left(\frac{A}{2}\right)^{2(s+1)}\frac{\Gamma(k-s+1)(s+3)(\Gamma(s+4))^2}{\Gamma(k+s-1)}\\ &\quad\times (C_f)^2(d_f)^{2s+6}.\end{aligned}$$

We select now $k = p_j$ and $s = \alpha_j p_j$ with $0 < \alpha_j < 1$ still at our disposal and obtain

$$\inf_\pi \|f-\pi\|^2_{L^\infty(K_{i,j})} \le C(x_1^j)^{-2-2\beta}\left(\frac{A}{2}\right)^{2(s+1)}\Theta(\alpha_j,p_j)(C_f)^2(d_f)^{2s+6}$$

where

$$\Theta(\alpha,p) = \frac{\Gamma((1-\alpha)p+1)(3+\alpha p)(\Gamma(4+\alpha p))^2}{\Gamma((1+\alpha)p-1)}.$$

step 3: For fixed $\alpha \in (0,1)$ and $p \in \mathbb{N}$ we claim that

$$\Theta(\alpha,p) \le Cp^{10}\left(\frac{(1-\alpha)^{1-\alpha}}{(1+\alpha)^{1+\alpha}}\right)^p\alpha^{2\alpha p} \tag{4.11}$$

where the constant C is independent of α and p. To show (4.11), we recall Stirling's formula

$$n! \sim \left(\frac{n}{e}\right)^{n+1/2}, \qquad n\to\infty$$

where $\sim$ indicates proportionality up to terms of lower order in n. With $s = \alpha p$ we have, as $p \to \infty$, that

$$\Theta(\alpha, p) \sim \frac{(p-s)!(s+3)((s+3)!)^2}{(p+s-2)!}$$
$$\sim \frac{((1-\alpha)p)^{(1-\alpha)p+1/2} e^{-(1-\alpha)p} (3+\alpha p)^{8+2\alpha p} e^{-6-2\alpha p}}{((1+\alpha)p-2)^{(1+\alpha)p-3/2} e^{-(1+\alpha)p+2}}.$$

Now

$$\left(1 - \frac{2}{(1+\alpha)p}\right)^{2((1+\alpha)p/2)} \to e^{-2} \qquad p \to \infty$$

and

$$(3+\alpha p)^{2\alpha p}(\alpha p)^{-2\alpha p} = \left(1 + \frac{3}{\alpha p}\right)^{6(\alpha p/3)} \to e^{6} \qquad p \to \infty$$

so that

$$\Theta(\alpha, p) \le C p^{10} \left(\frac{(1-\alpha)^{1-\alpha}}{(1+\alpha)^{1+\alpha}}\right)^{p} p^{-2\alpha p} (\alpha p)^{2\alpha p}$$

which proves (4.11).

step 4: Define

$$\varrho := \max\left\{\frac{3}{d_f}, \frac{1-\sigma}{\sigma}\right\}. \tag{4.12}$$

Then we have from Remark 4.1 that $\Lambda \le \varrho$ and

$$\inf_{\pi} \|f - \pi\|^2_{L^\infty(K_{i,j})} \le C(x_1^j)^{-2-2\beta} \varrho^{2\alpha p_j+2} (C_f)^2 (d_f)^6 p_j^{10} |F(\varrho d_f, \alpha_j)|^{2p_j}$$

where

$$F(x,\alpha) = \left(\frac{(1-\alpha)^{1-\alpha}}{(1+\alpha)^{1+\alpha}}\right)^{1/2} \left(\frac{x\alpha}{2}\right)^{\alpha} : [0,\infty) \times (0,1) \to \mathbb{R}.$$

Since

$$|K_{i,j}| = (h_j)^2 = (x_1^j)^2 (1-\sigma)^2,$$

we find for $1 \le i \le 3$, $2 \le j \le n+1$ that

$$|K_{i,j}| \inf_{\pi} \|f - \pi\|_{L^\infty(K_{i,j})} \le C(x_1^j)^{1-\beta} \varrho p_j^5 |F(\varrho d_f, \alpha_j)|^{p_j} C_f (d_f)^3.$$

step 5 (discussion of $F(x,\alpha)$): Obviously

$$\left|F\left(\frac{2}{z}, z\right)\right|^2 = \frac{(1-z)^{1-z}}{(1+z)^{1+z}} < 1 \qquad \text{for} \quad 0 < z < 1.$$

Due to (4.12) we have $2/(\varrho d_f) \leq 2/3$ and therefore

$$F_{min} := \min_{\alpha \in (0,1)} F(\varrho d_f, \alpha) = F(\varrho d_f, \alpha_{min}) \leq F(\varrho d_f, 2/(\varrho d_f)) < 1 \quad (4.13)$$

where

$$0 < \alpha_{min} = 2/(4 + (\varrho d_f)^2)^{1/2} = 2 \bigg/ \left(4 + \left(\max\left(3, \frac{1-\sigma}{\sigma} d_f\right)\right)^2\right)^{1/2} < 1.$$

step 6: Combining the above estimates, we get with (3.1)

$$|E_\sigma^{n,\mathbf{p}} f| \leq C C_f \left\{ \sigma^{(1-\beta)n} + \sum_{j=2}^{n+1} \sigma^{(n+1-j)(1-\beta)} p_j^5 |F_{min}|^{p_j} (d_f)^3 \right\} \quad (4.14)$$

where we selected $\alpha_j = \alpha_{min}$ for $2 \leq j \leq n+1$. Next, we choose a *linear degree vector* (4.1) where the slope μ satisfies

$$\mu = (1-\beta)\ln(\sigma)/\ln(F_{min}) + \varepsilon \quad (4.15)$$

for some $\varepsilon > 0$. Define

$$j_0 = \max\{j: 2 \leq j \leq n+1, \lfloor j\mu \rfloor \leq 1\}$$

and set $j_0 = 1$ if the set is empty. Then, using that $d_f \geq 1$,

$$|E_\sigma^{n,\mathbf{p}} f| \leq C(\beta,\sigma) C_f (d_f)^3 \sigma^{(n+1)(1-\beta)} \left\{ 1 + \sum_{j=2}^{j_0} \frac{2^5 |F_{min}|^2}{\sigma^{j(1-\beta)}} + \sum_{j=j_0+1}^{n+1} (\lfloor j\mu \rfloor + 1)^5 (F_{min})^{j\varepsilon} \right\}$$

where the curved parentheses depend on ε, μ, σ, β and α_{min}, but are bounded independently of n and C_f since $F_{min} < 1$ (cf. (4.13)) and $j_0 \leq 2/\mu$. Thus we obtain

$$|E_\sigma^{n,\mathbf{p}} f| \leq C(\sigma, \beta, d_f, \mu) C_f \sigma^{(1-\beta)(n+1)}. \quad (4.16)$$

step 7: We estimate the number N of quadrature points in $Q_\sigma^{n,\mathbf{p}}$ in dependence on n. For interpolatory rules, we need at most $(p_j+1)^2$ points in $K_{i,j}$. Hence

$$N \leq 3 \sum_{j=1}^{n+1} (p_j+1)^2 \leq \frac{54}{\mu} + (n+1)^3(\mu^2 + 6\mu + 12)$$

from where we find that

$$(n+1)^3 \geq \frac{N}{\mu^2 + 6\mu + 12} - \frac{54}{\mu(\mu^2 + 6\mu + 12)}.$$

Inserting this in (4.16) yields (4.3) and completes the proof. □

Remark 4.2. Theorem 4.1 holds in particular in the important case $\sigma = 0.5$, i.e. for partitions K_σ^n that are obtained by successive bisections which are often generated in adaptive integrators. As we will show in the numerical experiments in Section 6 below, however, the value $\sigma = 0.5$ is far from optimal for integrands from the class $\mathscr{B}_\beta(K)$.

Another important case of Theorem 4.1 occurs when the degree vector is *uniform*, i.e. $p_2 = p_3 = \cdots = p_{n+1} = p$.

Corollary 4.1. *For composite quadratures* $Q_\sigma^{n,\mathbf{p}}$ *of* uniform *order* $p = \lfloor \mu(n+1) \rfloor$ *for some* $\mu > 0$ *the estimate* (4.3) *holds without the assumption* (4.2).

Remark 4.3. So far we considered only the case where $O \in \bar{K}$. In this case (4.16) shows that it is essential to let the number n of layers tend to infinity as N increases. If the singular point O is located in the exterior of $\bar{K}$, n can be kept fixed and we obtain the convergence rate $\exp(-bN^{1/2})$ as $\min_{1 \le j \le n+1}\{p_j\} \to \infty$.

5. Generalizations

The exponential convergence result in Theorem 4.1 and its proof admit several generalizations, since its main components, a subdivision Ω_σ^n of the integration domain Ω that is geometrically graded towards the singular point O and a family $\mathcal{Q}$ of PI rules can be constructed in various cases. We consider first the simplex $T = \{(x_1, x_2) | 0 < x_1 < 1, 0 < x_2 < x_1\} \subset \mathbb{R}^2$ and $O = (0,0)$. With x_1^j and x_2^j as in (3.1), we define the domains

$$T_1 = \{(x_1, x_2) | 0 < x_1 < \sigma^n, 0 < x_2 < x_1\}$$

$$T_j = \{(x_1, x_2) | x_1^{j-1} < x_1 < x_1^j, 0 < x_2 < x_1^{j-1} + x_1\} \qquad j = 2, \dots, n+1$$

The subdivision of T with $n+1$ layers is denoted by T_σ^n and Fig. 2 depicts $T_{0.5}^3$. In particular, the domains T_j for $j \ge 2$ are scaled images of the reference domain

$$\hat{T} = \{(x_1, x_2) | 1 < x_1 < 2, 0 < x_2 < x_1\}.$$

for $j \ge 2$. In the design of the composite rule $Q_\sigma^{n,\mathbf{p}}$ a family $\mathcal{Q} = \{Q^{p_i}\}$ of rules which are exact of total degree p_i on $\hat{T}$ is needed. The following lemma shows how to construct such a family from a one dimensional PI family for $(0,1)$, such as for example the Gauss-Legendre family.

Lemma 5.1. *Let* $\mathcal{G} = \{G^p\}$ *be a family of one dimensional PI quadratures of degrees* $p = 1, 2, \dots$ *on* $(0,1)$ *with weights* $w_i^{(p)}$ *and knots* $z_i^{(p)}$. *Then the family* $\mathcal{Q} = \{Q^p\}$ *of rules which are defined by*

$$Q^p f = \sum_i \sum_j w_i^{(2p+1)} w_j^{(p)} z_i^{(2p+1)} f(1 + z_i^{(2p+1)}, z_j^{(p)}(1 + z_i^{(2p+1)})) \tag{5.1}$$

are exact for all polynomials of total degree p *on* $\hat{T}$.

Proof: The assertion is a consequence of the Duffy transformation

$$\int_1^2 \int_0^{x_1} f(x_1, x_2)\, dx_1\, dx_2 = \int_1^2 \int_0^1 f(y_1, y_1 y_2) y_1\, dy_1\, dy_2\,. \tag{5.2}$$

□

Remark 5.1. The transformation (5.2) is known to remove singularities of integrands which are homogeneous of degree -1 in $|x|$ in the sense that the integrand on the right hand side of (5.2) is an analytic function of (y_1, y_2) on $\overline{(1,2) \times (0,1)}$ [12]. This, however, is not the case for degrees of homogeneity other than -1.

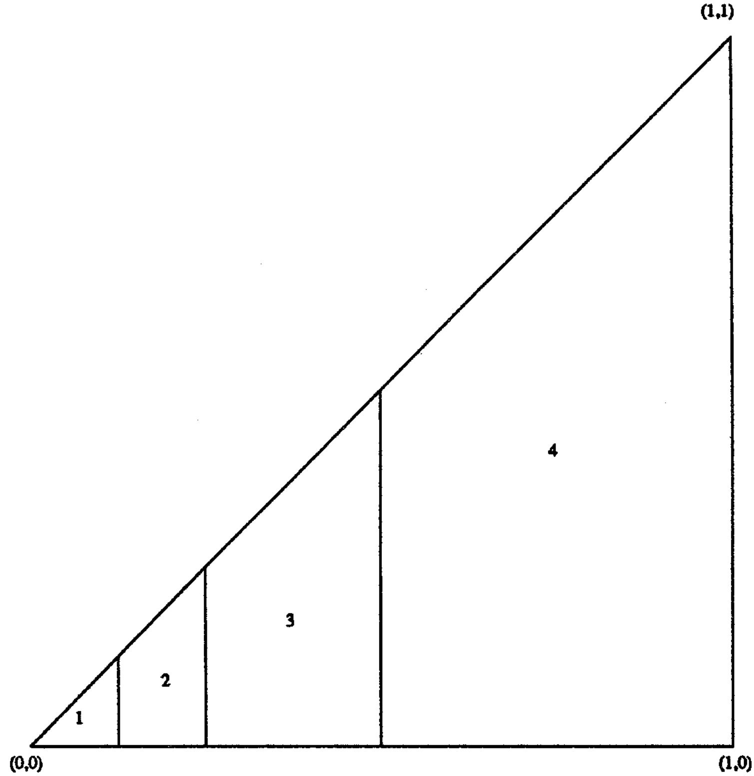

Figure 2. Geometric subdivision T_σ^n with $n = 3$ and $\sigma = 0.5$

For the unit simplex, a proof quite analogous to that of Theorem 4.1 yields

Theorem 5.1. *Let $T \subset \mathbb{R}^2$ denote the unit simplex and assume that $f \in \mathscr{B}_\beta(T)$. Let $Q_\sigma^{n,\mathbf{p}}$ denote a composite quadrature rule with the linear degree vector* (4.1) *corresponding to the geometric partition T_σ^n of T with $0 < \sigma < 1$. Then there exists a constant $b > 0$ independent of N such that*

$$\left| \int_T f(x)\,dx - Q_\sigma^{n,\mathbf{p}} f \right| \leq C C_f \exp(-bN^{1/3}) \tag{5.3}$$

where C depends on σ, β, μ, d_f and C_f and d_f are the constants in (2.2).

We consider next the quadrature of functions $f \in \mathscr{B}_\beta(K)$ over the unit cube $K \in \mathbb{R}^r$ in dimensions other than 2. Once again geometric subdivisions K_σ^n like the one in Fig. 1 can be defined. They consist now of $K_{1,1}$ and n layers of $2^r - 1$ scaled hypercubes each. The construction of the composite quadratures $Q_\sigma^{n,\mathbf{p}}$ is based on properly scaled, r-fold tensor products of PI rules on $(0, 1)$.

Many ingredients of the convergence analysis of Theorem 4.1 have already been proved for dimensions $r \neq 2$. The only genuinely two dimensional result used was

Proposition 4.1; provided, an analogous result holds also in dimensions $r > 2$ (for $r = 1$ this is fairly straightforward to show), we have the following generalization of (4.3).

$$\left| \int_K f(x)\,dx - Q_\sigma^{n,\mathbf{p}} f \right| \leq CC_f \exp(-bN^{1/(r+1)}) \qquad \forall 0 < \sigma < 1, f \in \mathscr{B}_\beta(K) \quad (5.4)$$

provided a linear degree vector (4.1) is used. Here the constants C and b depend also on the dimension r, but are independent of the number of integrand evaluations N.

Remark 5.2. The estimate (5.4) for $r = 1$ and special integrands $f(x) = x^\alpha g(x)$ with $\alpha > 0$ and a function $g(x)$ which is analytic in [0, 1] is a straightforward consequence of Lemma 4.1 and [10, Theorem 3] as we observed in [11]. Since the class $\mathscr{B}_\beta(K)$, however, contains functions of the form $f(x) = x^\alpha g(x)$ with $\alpha > -1$, (5.4) for $r = 1$ already generalizes [10].

Remark 5.3. Since our convergence proof used arguments from approximation theory, exponential convergence results can also be obtained for curved regions of integration Ω and curved subdomains in Ω^n, analogous to what is done in the $h - p$ version of the finite element method (see [4, Part 2] for details and explicit constructions of analytic domain mappings).

Remark 5.4. Another generalization of variable order composite quadrature addresses integrands which become singular anisotropically along a line, as e.g.

$$f(x_1, x_2) = x_1^\alpha g(x_1, x_2)$$

where g is a smooth function. Now tensor products of variable order, composite quadratures in x_1 with high order Gaussian quadrature in x_2 yield again exponential convergence. This is true also for integrands in classes $\mathscr{B}_\beta(\Omega)$ with anisotropic weight functions Φ—since the main ideas of the proof are similar and the details are lengthy, we will not elaborate on them.

6. Numerical Examples

In this section we present numerical examples which show that the exponential convergence rate (1.1) is sharp. All computations were done in double precision FORTRAN at the IBM Scientific Centre, Heidelberg.

We consider first the case $K = (0, 1)$ and $f = x^{-1/2}$ which belongs to $\mathscr{B}_\beta(K)$ for $\beta > 0$ according to Proposition 2.1. Figure 3 depicts the decadic logarithm of the relative quadrature error for the composite quadrature with linear degree vector versus $\sqrt{N}$ for various values of σ. According to the estimate (5.4) with $r = 1$ we expect a linear dependence of these quantities. The component rules were obtained from the Gauss-Legendre family and the degree vector was again linear with slope $\mu = 1$. The optimal grading factor σ appears to be very close to 0.15 in accordance with the optimal value $\sigma = (\sqrt{2} - 1)^2 \sim 0.17\ldots$ obtained by K. Scherer [10] in a closely

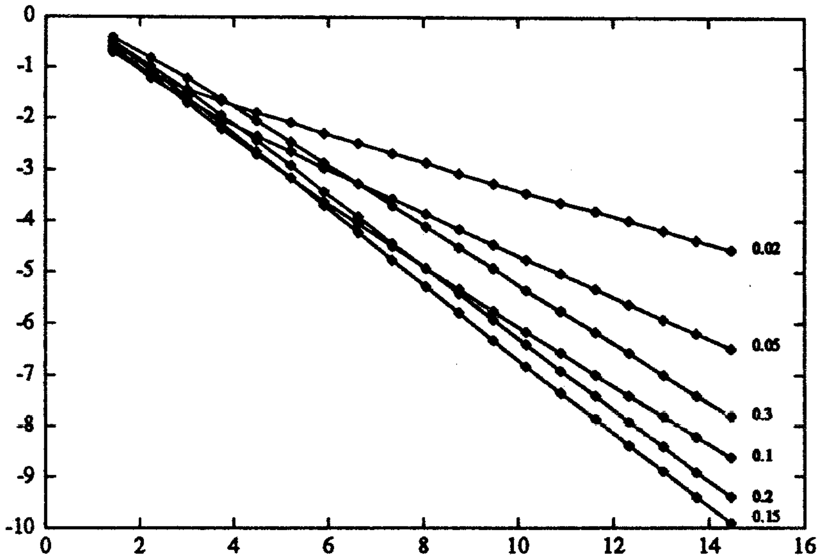

Figure 3. $\log_{10}(|Ef|/|If|)$ versus $N^{1/2}$ for $f(x) = x^{-1/2}$ and various σ

related problem of best approximation. We observe that the estimate (5.4) for $r = 1$ is already sharp for small values of N. We considered next examples with a two-dimensional integral domain In Fig. 4 we show the relative quadrature error for

$$\int_0^1 \int_0^{x_1} \frac{1}{\rho^{3/2}} dx_1\, dx_2 \tag{6.1}$$

using the composite rules $Q_\sigma^{n,\mathbf{p}}$ based on a family $\mathcal{Q}$ as in Lemma 5.1 with the family $\mathcal{G}$ of Gauss-Legendre rules on (0, 1) and a linear linear degree vector (4.1) with slope $\mu = 1$. By Proposition 2.2, the integrand belongs to $\mathcal{B}_\beta(T)$ for $\beta > 1/2$. The optimal grading parameter σ for $\mu = 1$ seems to be near $\sigma = 0.025$. The validity of the error estimate (5.3) is apparent already for small values of N.

So far we considered only integrands of the form singularity times a smooth (analytic) function. For such integrands special, weighted quadratures can be developed which will outperform the composite rules $Q_\sigma^{n,\mathbf{p}}$, since their rate of convergence is governed by the polynomial approximability of the smooth function. Theorem 4.1 and its generalizations however, ensure *uniform* exponential convergence of the composite quadratures on a family $\mathcal{F} \subset \mathcal{B}_\beta$ of integrands. Such families arise, for example, in the boundary element method (BEM) where almost singular integrals have to be evaluated. Here the singular point is outside in a distance ε to the domain of integration and one needs a method that is uniformly accurate in ε. In particular, the exact location of the source point in the integration coordinates is, as a rule, not known explicitly.

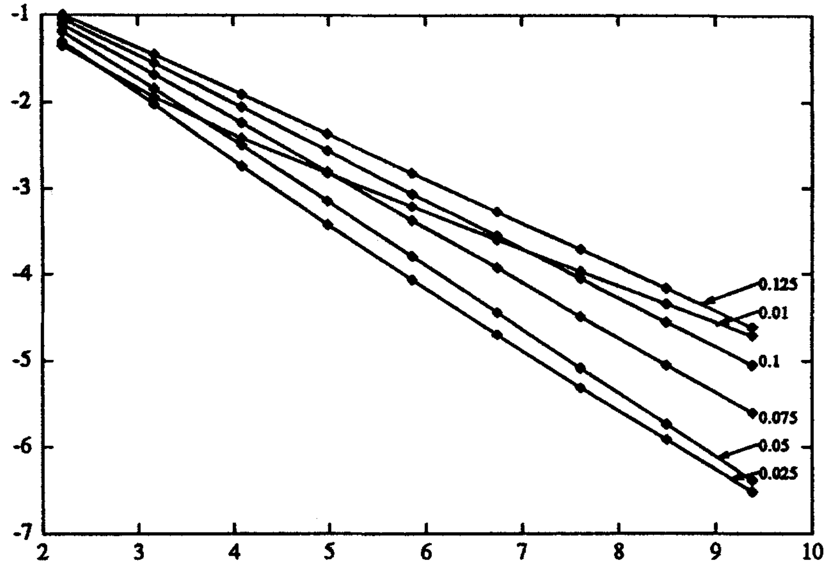

Figure 4. $\log_{10}(|Ef|/|If|)$ versus $N^{1/3}$ for $f(x) = |x|^{-3/2}$ and various σ

As a model integral, consider the single layer potential integral

$$I_\varepsilon^{SLP} = \int_K \frac{1}{|x-y|} dy \tag{6.2}$$

where $x = (0, 0, \varepsilon)^t$ and $y = (y_1, y_2, 0)^t$. Note that in local polar coordinates in the (y_1, y_2)-plane

$$\frac{1}{|x-y|} = (\varepsilon^2 + \rho^2)^{-1/2} \in \mathscr{B}_\beta(K) \qquad \text{if } \beta > 0 \quad \text{and} \quad \varepsilon = 0 .$$

According to Theorem 4.1, we expect therefore exponential convergence regardless of the value of ε. Figure 5 shows the decimal logarithm of the relative quadrature error versus $N^{1/3}$ for $\mu = 0.5$, $\sigma = 0.15$ and several values of ε. We clearly see that for small ε the exponential convergence rate $\exp(-bN^{1/3})$ is attained, whereas for $\varepsilon = 1.0$ the curve seems to bend downward due to the expected convergence rate of $\exp(-bN^{1/2})$ (cf. Remark 4.3). Consequently, the performance of the composite quadratures is *robust* with respect to the distance of the source point to K.

Finally, to illustrate the limitations of the method, we consider the almost singular double layer potential which arises together with (6.2) in the evaluation of the representation formula for source points near to the boundary of the domain, i.e.

$$I_\varepsilon^{DLP} = \int_K \frac{\vec{n}(y) \cdot (x-y)}{|x-y|^3} dy = \operatorname{sign}(\varepsilon)\frac{\pi}{2} - 2 \arcsin\left(\frac{\varepsilon\sqrt{2}}{2\sqrt{1+\varepsilon^2}}\right) \tag{6.3}$$

where $x = (0, 0, \varepsilon)^t$, $y = (y_1, y_2, 0)^t$ and $\vec{n}(y) = (0, 0, 1)^t$. This potential exhibits as is

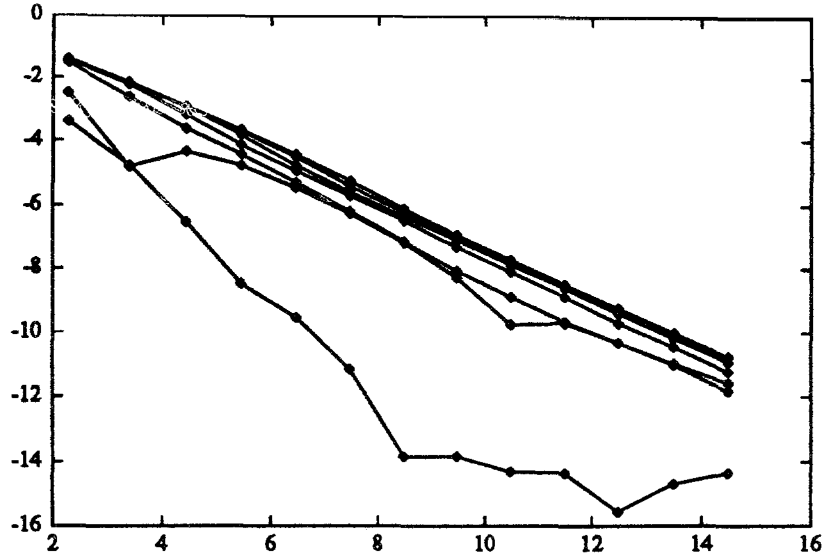

Figure 5. $\log_{10}(|Ef|/|I_\varepsilon^{SLP}|)$ versus $N^{1/3}$ for $\sigma = 0.15$ and $\varepsilon = 10^{-j}$, $j = 0, \ldots, 6$

well known, a jump when the source point x passes through the plane $x_3 = 0$ or, equivalently, as ε changes sign. In Fig. 6 we display the performance of the composite quadratures $Q_\sigma^{n,\mathbf{p}}$ with linear degree vector (4.1), slope $\mu = 1/2$ and $\sigma = 0.15$ for various values of ε. The family of integrands does not belong uniformly to $\mathscr{B}_\beta(K)$ for any $0 < \beta < 1$ and the performance of the composite quadrature deteriorates as the source point approaches the surface. Nevertheless, in a wide range of ε the results are still acceptable. This is in a sense the best one can expect with a purely numerical method. To obtain here results which are accurate to machine precision, one must use series expansions of the potentials and their explicit one-sided jump relations which we will investigate in a forthcoming paper [14].

7. Appendix

In this section, we will prove Proposition 2.2. To this end, we must verify (2.2).

The growth condition (2.2) on the derivatives of $f \in \mathscr{B}_\beta(\Omega)$ is expressed via derivatives of f Cartesian coordinates. Occasionally, however, the following alternative characterization via derivatives in polar coordinates of f is useful.

Proposition A.1 [2]. *Let $\Omega \subset \mathbb{R}^2$ and $O \in \Omega$. Denote the polar coordinates at O by (r, θ) and, for $\alpha \in \mathbb{N}_0^2$,*

$$\mathscr{D}^\alpha f = \frac{\partial^{|\alpha|} f}{\partial r^{\alpha_1} \partial \theta^{\alpha_2}}.$$

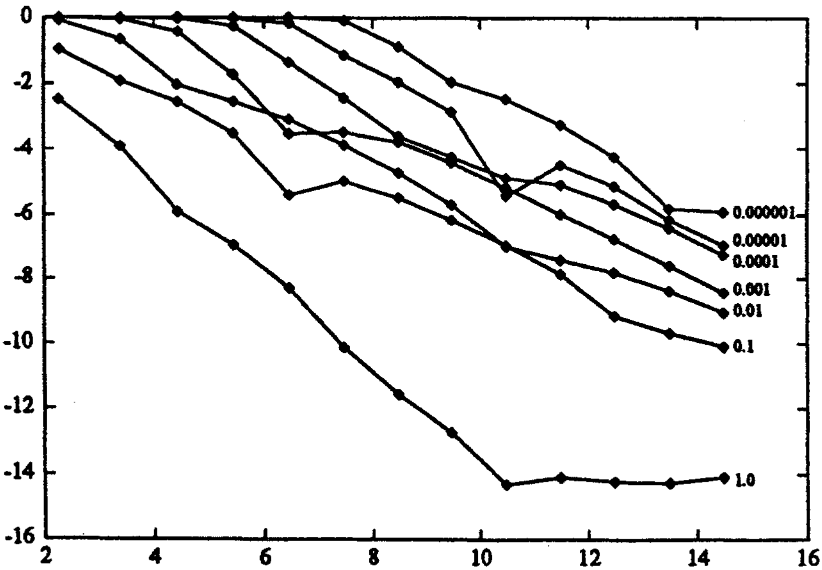

Figure 6. $\log_{10}(|Ef|/|I_\varepsilon^{DLP}|)$ vesus $N^{1/3}$ for $\sigma = 0.15$ and $\varepsilon = 10^{-j}$, $j = 0,\ldots,6$

Then (2.2) *holds if and only if there exist constants* $\tilde{C}_f$ *and* $\tilde{d}_f$ *(possibly different from* C_f, d_f*) that are independent of k so that*

$$\left(\int_\Omega |\mathscr{D}^\alpha f|^2 r^{2(k+\beta-\alpha_2)} r\,dr\,d\theta\right)^{1/2} \le \tilde{C}_f(\tilde{d}_f)^k k! \qquad \forall |\alpha| = k \in \mathbb{N}_0. \tag{A.1}$$

Since $f_\varepsilon(r) = (\varepsilon + r)^\lambda$ is a radial function, this proposition shows we must only estimate the growth of derivatives with respect to r in order to prove Proposition 2.2.

Since $\lambda < 0$ and

$$\frac{\partial^k f_\varepsilon(r)}{\partial r^k} = \lambda(\lambda - 1)(\lambda - 2)\ldots(\lambda - k + 1)(\varepsilon + r)^{\lambda - k},$$

we have with $\alpha = (k, 0)$ that

$$\begin{aligned}\int_K |\mathscr{D}^\alpha f_\varepsilon(r)|^2 r^{2(k+\beta-\alpha_2)} r\,dr\,d\theta &\le ((k+1)!)^2 \int_0^{\pi/4}\int_0^{\sqrt{2}} (\varepsilon + r)^{2(\lambda-k)} r^{2k+2\beta+1}\,dr\,d\theta \\ &\le \frac{\pi}{4}(k+1)^2(k!)^2 \int_0^{\sqrt{2}} r^{2\lambda-2k+2k+2\beta+1}\,dr \\ &= \frac{\pi}{4}\frac{2^{\lambda+\beta+1}}{2\lambda+2\beta+2} 2^{2k}(k!)^2.\end{aligned}$$

This is (A.1) with

$$\tilde{d}_f = 2 \qquad \text{and} \qquad (\tilde{C}_f)^2 = \frac{\pi}{4}\frac{2^{\lambda+\beta+1}}{2(\lambda+\beta+1)},$$

provided that $\beta + \lambda + 1 > 0$. Proposition 2.2 is now a consequence of Proposition A.1.

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