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Published Version

Chernov, A. and Schwab, C. (2012) Exponential convergence of Gauss--Jacobi quadratures for singular integrals over simplices in arbitrary dimension. SIAM Journal on Numerical Analysis (SINUM), 50 (3). pp. 1433-1455. ISSN 0036-1429 doi: https://doi.org/10.1137/100812574 Available at https://centaur.reading.ac.uk/33216/

SIAM J. NUMER. ANAL.
Vol. 50, No. 3, pp. 1433–1455

EXPONENTIAL CONVERGENCE OF GAUSS–JACOBI QUADRATURES FOR SINGULAR INTEGRALS OVER SIMPLICES IN ARBITRARY DIMENSION*

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Abstract. Galerkin discretizations of integral operators in $\mathbb{R}^d$ require the evaluation of integrals $\int_{S^{(1)}}\int_{S^{(2)}} f(x,y)\,dydx$, where $S^{(1)}, S^{(2)}$ are d-dimensional simplices and f has a singularity at $x = y$. In [A. Chernov, T. von Petersdorff, and C. Schwab, *M2AN Math. Model. Numer. Anal.*, 45 (2011), pp. 387–422] we constructed a family of hp-quadrature rules Q_N with N function evaluations for a class of integrands f allowing for algebraic singularities at $x = y$, possibly nonintegrable with respect to either dx or dy (hypersingular kernels) and Gevrey-δ smooth for $x \neq y$. This is satisfied for kernels from broad classes of pseudodifferential operators. We proved that Q_N achieves the exponential convergence rate $\mathcal{O}(\exp(-rN^\gamma))$ with the exponent $\gamma = 1/(2d\delta + 1)$. In this paper we consider a special singularity $\|x - y\|^\alpha$ with real α which appears frequently in appplication and prove that an improved convergence rate with $\gamma = 1/(2d\delta)$ is achieved if a certain one-dimensional Gauss–Jacobi quadrature rule is used in the (univariate) "singular coordinate." We also analyze approximation by tensor Gauss–Jacobi quadratures in the "regular coordinates." We illustrate the performance of the new Gauss–Jacobi rules on several numerical examples and compare it to the hp-quadratures from [A. Chernov, T. von Petersdorff, and C. Schwab, *M2AN Math. Model. Numer. Anal.*, 45 (2011), pp. 387–422].

Key words. Gauss–Jacobi quadrature, numerical integration, high dimensional integrands, hypersingular integrals, integral equations, Gevrey regularity, exponential convergence

AMS subject classifications. 65N30, 65D30, 32A55

DOI. 10.1137/100812574

1. Introduction and notation. A basic problem in the numerical analysis of Galerkin discretizations of singular integral equations involves computation of double integrals of the type

$$\int_{x\in\Omega_{\mathrm{op}}}\int_{y\in\Omega_{\mathrm{op}}} K(x,y)\phi_j(y)\phi_i(x)\,dydx.$$

Here, the set Ω_{op} denotes the domain of definition of the pseudodifferential operator with Schwartz kernel $K(x,y)$. Typically, the kernel $K(x,y)$ is smooth for $x \neq y$ but becomes strongly singular at $x = y$ [6, 13]. In this case, integration with respect to $K(x,y)$ must be interpreted in a suitable sense; cf., e.g., [9]. In finite element type Galerkin discretizations, the functions ϕ_j are piecewise polynomials on closed simplices. Then, this amounts to computing integrals of the type

$$I = \int_{x\in S^{(1)}}\int_{y\in S^{(2)}} K(x,y)\phi_j(y)\phi_i(x)\,dydx, \tag{1.1}$$

where $S^{(1)}, S^{(2)}$ are closed simplices of the mesh and the restrictions $\phi_i|_{S^{(1)}}$, $\phi_j|_{S^{(2)}}$ are smooth functions in $S^{(1)}$, $S^{(2)}$. If the simplices touch or coincide, the integrand is singular. Throughout, we work under an assumption of shape regularity of $S^{(1)}, S^{(2)}$.

*Received by the editors October 22, 2010; accepted for publication (in revised form) January 23, 2012; published electronically June 5, 2012.
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Assumption 1. For closed simplices $S^{(1)}, S^{(2)}$ in $\mathbb{R}^d$ let $h_j := \operatorname{diam} S^{(j)}$ denote the diameters, and let ρ_j denote the radii of the largest ball contained in $S^{(j)}$ for $j = 1, 2$. The simplices $S^{(1)}, S^{(2)}$ are shape regular in the following sense: There exist $C_1, C_2 > 0$ with

$$\frac{h_j}{\rho_j} \le C_1.$$

If $S^{(1)} \cap S^{(2)}$ is empty, then we let $k := -1$ and assume

$$\operatorname{dist}(S^{(1)}, S^{(2)}) \ge C_2^{-1} \max\{h_1, h_2\}.$$

If $S^{(1)} \cap S^{(2)}$ is nonempty, the intersection is the convex hull of $k+1$ vertices of $S^{(j)}$ for $j = 1, 2$ with $k \in \{0, \dots, d\}$. We assume that $S^{(1)}, S^{(2)}$ are nondegenerate in the sense that the matrices $A^{(j)}$, $B^{(j)}$ defined in Step 1 below are uniformly nondegenerate.

These assumptions are satisfied if $S^{(1)}, S^{(2)}$ are part of a shape regular finite element mesh. Note that this condition is preserved under regular mesh refinements. The convergence estimate of the type (1.6) below will hold for any values C_j, but the constants will deteriorate for large values of C_j.

If the original domain of definition Ω_{op} is curved or consists of a piecewise analytic or Gevrey-δ regular manifold in a higher dimensional space (e.g., the boundary of a polyhedron in $\mathbb{R}^{d+1}$), the functions $\phi_i|_{S^{(1)}}$ and $\phi_j|_{S^{(2)}}$ might include parametric mappings, Jacobians, and cutoff functions but are still Gevrey-δ regular functions on $S^{(1)}$ and $S^{(2)}$ (cf. Proposition A.2 in the appendix) in the following sense.

DEFINITION 1.1. *Let $\Omega \subset \mathbb{R}^m$ be a closed bounded set, and let $\delta \ge 1$. A function $f : \Omega \to \mathbb{R}$ is Gevrey-δ regular $f \in G^\delta(\Omega)$ iff there exist $A_0, A_1 > 0$ so that*

$$|D^\nu f(x)| \le A_0 A_1^{|\nu|} (\nu!)^\delta \qquad \forall x \in \Omega, \quad \forall \nu \in \mathbb{N}_0^m. \tag{1.2}$$

A vector-valued $f \in G^\delta(\Omega)$ if (1.2) *holds for every component of f.*

We remark that for $\delta = 1$, Gevrey regularity implies analyticity. The case $\delta > 1$ corresponds to nonanalytic but smooth classes of functions. We refer the reader to [1, 3] for more details on Gevrey classes $G^\delta(\Omega)$ for $\delta > 1$.

In all these cases the integrand can be written as a function $F(x, y, y - x) \in L^1(S^{(1)} \times S^{(2)})$, where $F(x, y, z)$ is Gevrey-δ regular in x, y, z for $z \ne 0$ but might have a singularity at $z = 0$. Precisely, the integral I from (1.1) takes the form

$$I = \int_{x \in S^{(1)}} \int_{y \in S^{(2)}} F(x, y, y - x)\, dy dx, \tag{1.3}$$

and F satisfies the following assumption.

Assumption 2. There exist $\alpha > k - 2d$, $A_0, A_1 > 0$, and $\delta \ge 1$ so that for all $\nu = (\nu_x, \nu_y, \nu_z) \in \mathbb{N}_0^{3d}$, $x \in S^{(1)}$, $y \in S^{(2)}$, and $z \in S^{(2)} - S^{(1)}$,

$$|D^\nu F(x, y, z)| \le A_0 A_1^{|\nu|} (\nu!)^\delta \, \|z\|^{\min(\alpha - |\nu_z|, 0)}. \tag{1.4}$$

The parameter α is termed the order of singularity.

Our aim is to approximate the singular integral I from (1.3) by a quadrature rule,

$$Q_N = \sum_{\lambda=1}^{N} F(x_\lambda, y_\lambda, z_\lambda) w_\lambda, \tag{1.5}$$

with the quadrature nodes $(x_\lambda, y_\lambda, z_\lambda) \in S^{(1)} \times S^{(2)} \times (S^{(2)} - S^{(1)}) \setminus \{0\}$ and positive quadrature weights w_λ.

Remark 1. In exact arithmetic $z_\lambda = y_\lambda - x_\lambda$, and the intermediate storage of z_λ is redundant in an implementation. In the finite precision, float point arithmetic, evaluation of the difference $y_\lambda - x_\lambda$ in general is susceptive to subtractive cancellation. This effect was pointed out in [3, Remark 3.7] and is illustrated on a numerical example in [3, Figure 5]. To avoid such subtractive cancellation, we propose keeping z_λ and using transformations avoiding subtractive cancellation. This is the reason for (3.15).

In [3] we constructed a family of *hp*-quadrature (or "variable-order, composite") rules Q_N of the form (1.5) and proved the exponential convergence with respect to N:

$$|I - Q_N| \le C \exp(-rN^\gamma) \tag{1.6}$$

with $r > 0$ independent of N and d and the exponent $\gamma = 1/(2d\delta + 1)$. An improved convergence rate with $\gamma = 1/(2d\delta)$ is achieved if $k = -1$ (no singularity) or when $\alpha > k - 2d$ is an integer. Our construction consists of a sequence of analytic, regularizing coordinate transforms which *reduce the dimensionality of the singularity* and, at the same time, simplify the domain of integration. In particular, we prove here that after this parameter transform the domain of integration is a cube $[0, 1]^{2d}$ and the singular support of the integrand is *univariate* while the integrand is Gevrey-δ regular in the remaining $2d - 1$ coordinates *with the same Gevrey exponent* δ.

In this paper we prove that the improved convergence rate (1.6) with $\gamma = 1/(2d\delta)$ can be achieved for a particular important class of integrands involving kernels of the type

$$F(x, y, z) = \|z\|^\alpha \tilde{F}(x, y, z). \tag{1.7}$$

Here $\alpha > k - 2d$ is a real number and $\tilde{F} \in G^\delta(S^{(1)} \times S^{(2)} \times (S^{(2)} - S^{(1)}))$ in the sense of Definition 1.1. In other words, this means that under assumption (1.7) our quadrature rule for singular integrands achieves asymptotically the *same precision* as a tensor Gauss–Legendre or Gauss–Jacobi quadrature rule for a Gevrey-δ integrand $\tilde{F}$ without singularity using the *same number of function evaluations*. This result has been known for integer α in dimension $d = 1, 2$ and for $\delta = 1$, which corresponds to layer or volume potentials related to elliptic PDEs; see Remark 4 and, e.g., [10, Chapter 5], [12]. Theorem 5.4 below extends this result to the case of general $d \ge 1$ and noninteger α. The main ingredient for this convergence result is Theorem 4.1, showing that for an integrand F satisfying (1.7), the transformed integrand has a singularity of the form $t_1^{\tilde{\alpha}}$ with $\tilde{\alpha} = \alpha + 2d - k - 1 > -1$. This can be treated as a weight of a one-dimensional Gauss–Jacobi quadrature rule on the interval $t_1 \in [0, 1]$. Clearly, in order to take advantage of this property, the singularity order α must be known, which was not required in [3] but is usually the case in applications.

The paper is organized as follows. In section 2 we introduce three basic classes of parametrizations of the reference simplex S_d which will be frequently used later on. In section 3 we describe Steps 1–8 of our coordinate transformations. Section 4 is dedicated to the detailed regularity analysis for integrands of the type (1.7). The convergence proofs justifying the improved convergence rates for the Gauss–Jacobi quadrature rules are given in section 5. In section 6 we give several numerical examples illustrating the improved convergence of the new Gauss–Jacobi $2d$-dimensional quadrature rules and compare it to the *hp*-quadratures from [3]. The appendix contains two technical propositions on the regularity of Gevrey-δ functions.

2. Basic parametrizations of the reference simplex. We adopt notation from [3]. Consider a subset $N = \{n_1, \dots, n_k\}$ of $\{1, \dots, d\}$ with $n_1 < \cdots < n_k$. For any $x \in \mathbb{R}^d$ we denote $x_N := (x_{n_1}, \dots, x_{n_k}) \in \mathbb{R}^k$ and $x^{(N)} \in \mathbb{R}^d$ by $x_j^{(N)} := x_j$ for $j \in N$, $x_j^{(N)} := 0$ for $j \notin N$. We write $x \geq 0$ for a vector x iff $x_j \geq 0$ for all j. For a finite set N we denote by $\#N$ the number of its elements. For $x \in \mathbb{R}^m$ we use the notation

$$\sigma_{(x_1,\dots,x_m)} = \sigma_x := \begin{cases} 1 - \sum_{j=1}^m x_j, & m \geq 1, \\ 1, & m = 0. \end{cases} \tag{2.1}$$

In this section we consider three basic analytic parametrizations of the reference simplex defined by

$$S_d := \{(x_1, \dots, x_d) \mid x \geq 0,\, x_1 + \cdots + x_d \leq 1\} \tag{2.2}$$

and the associate transformations of the integral over S_d

$$Y := \int_{x \in S_d} \varphi(x)\, dx \tag{2.3}$$

for some φ being integrable in S_d. The associated degenerate coordinate transforms will be frequently used in the regularizing coordinate transforms in section 3.

2.1. First parametrization of $x \in S_d$ by $(t, y) \in S_{d-k} \times S_k$. Definition (2.2) directly yields the parametrization

$$\begin{aligned} S_d &= \left\{x \mid 0 \leq x_j \leq \sigma_{(x_{j+1},\dots,x_d)}, 1 \leq j \leq d\right\} \\ &= \left\{x \mid (x_j, \dots, x_d) \in S_{d-j+1}, 1 \leq j \leq d\right\}. \end{aligned} \tag{2.4}$$

Let us fix some $k \in \{0, \dots, d\}$ and introduce the new variables t_j, y_j by recursion over the dimension:

$$t_j := x_{k+j}, \quad j = 1, \dots, d-k, \qquad \text{and} \qquad y_j := \frac{x_j}{\sigma_{(x_{k+1},\dots,x_d)}} = \frac{x_j}{\sigma_t}, \quad j = 1, \dots, k.$$

Then for $j = 1, \dots, k$ there holds

$$\begin{aligned} 0 \leq y_j = \frac{x_j}{\sigma_t} \leq \frac{1 - x_{j+1} - \cdots - x_d}{\sigma_t} = 1 - \frac{x_{j+1} + \cdots + x_k}{\sigma_t} &= 1 - y_{j+1} - \cdots - y_k \\ &= \sigma_{(y_{j+1},\dots,y_k)}; \end{aligned}$$

hence $y \in S_k$ and $t \in S_{d-k}$ due to (2.4). This yields the parametrization

$$S_d = \{(\sigma_t y, t) \mid t \in S_{d-k}, y \in S_k\}. \tag{2.5}$$

Inserting this parametrization into (2.3), we obtain

$$Y = \int_{t \in S_{d-k}} \int_{y \in S_k} \varphi(\sigma_t y, t) \sigma_t^k \, dy\, dt. \tag{2.6}$$

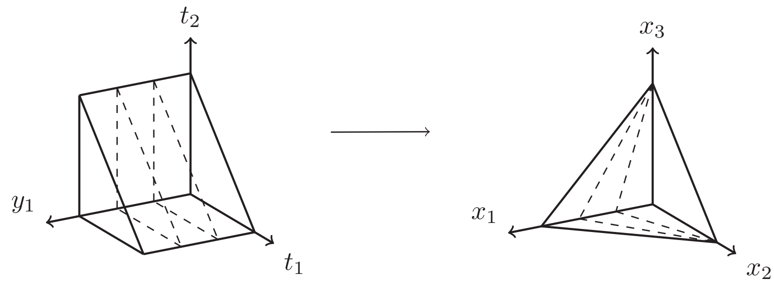

FIG. 2.1. *First parametrization* (2.5) *for* $d = 3$ *and* $k = 1$.

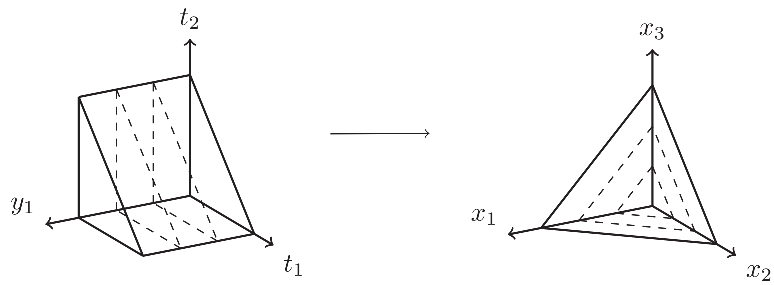

FIG. 2.2. *Second parametrization* (2.9) *for* $d = 3$.

2.2. Second parametrization of $x \in S_d$ by $(t, y) \in S_{d-1} \times [0, 1]$. Recall definition (2.2) of S_d. Then

$$B_d := \{(x_1, \dots, x_d) \mid x \geq 0,\, x_1 + \cdots + x_d = 1\} \tag{2.7}$$

is the face of S_d which does not include the origin $x = 0$. Basic calculations give alternative parametrizations of B_d and S_d:

$$B_d = \bigl\{(\sigma_t, t) \mid t \in S_{d-1}\bigr\}, \qquad S_d = \bigl\{y(x_1, \dots, x_d) \mid x \in B_d, y \in [0, 1]\bigr\}. \tag{2.8}$$

Their combination yields

$$S_d = \bigl\{(\sigma_t y, yt) \mid t \in S_{d-1}, y \in [0, 1]\bigr\} \tag{2.9}$$

and, upon inserting this into (2.3),

$$Y = \int_{t \in S_{d-1}} \int_{y \in [0,1]} \varphi(\sigma_t y, yt) y^{d-1}\, dy\, dt. \tag{2.10}$$

Note that (2.5) for $k = 1$ and (2.9) are two different parametrizations of S_d by $S_{d-1} \times [0, 1]$; see Figures 2.1 and 2.2.

2.3. Third parametrization of $x \in S_d$ by $t \in [0, 1]^d$. We introduce the following parametrization componentwise:

$$x_j = \chi_j(t) := \begin{cases} t_1 \dots t_j(1 - t_{j+1}), & j = 1, \dots, d - 1, \\ t_1 \dots t_d, & j = d. \end{cases} \tag{2.11}$$

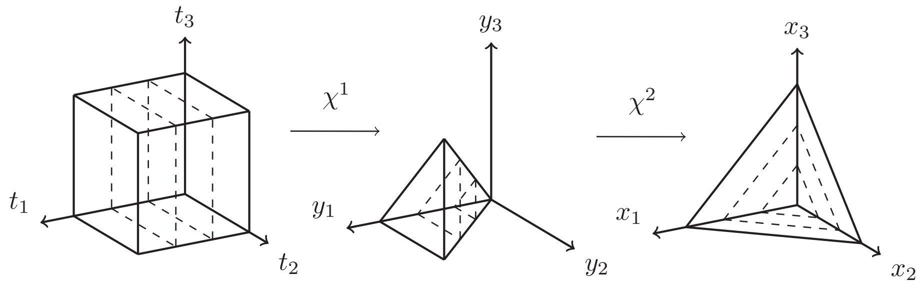

FIG. 2.3. *Third parametrization* (2.12) *for* $d = 3$.

We denote $\chi(t) := (\chi_1(t), \ldots, \chi_d(t))$. For an arbitrary $t \in [0,1]^d$ we obtain $0 \leq \sum_{j=1}^d \chi_j(t) = t_1 \leq 1$. This yields the parametrization

$$S_d = \{x = \chi(t) \mid t \in [0,1]^d\}. \tag{2.12}$$

We claim that the integral in (2.3) equals

$$Y = \int_{t \in [0,1]^d} \varphi(\chi(t)) J_\chi(t)\, dt, \qquad J_\chi(t) = t_1^{d-1} t_2^{d-2} \ldots t_{d-1}. \tag{2.13}$$

In order to show (2.13) we split $\chi = \chi^2 \circ \chi^1$, where

$$\chi_j^1(t) := t_1 \ldots t_j, \quad 1 \leq j \leq d, \qquad \chi_j^2(y) := \begin{cases} y_j - y_{j+1}, & 1 \leq j \leq d-1, \\ y_d, & j = d; \end{cases} \tag{2.14}$$

see Figure 2.3. Then

$$J_\chi(t) = \left|\det\left(\frac{\partial \chi}{\partial t}\right)\right| = \left|\det\left(\frac{\partial \chi^1}{\partial t}\right)\right| = t_1^{d-1} t_2^{d-2} \ldots t_{d-1}, \tag{2.15}$$

and (2.13) holds true.

3. Coordinate transformations. In this section we revisit coordinate transformations from [3], allowing us to rewrite (1.3) as an integral over a unit cube $[0,1]^{2d}$. Here, we introduce slightly different notation which is more convenient for the integrand functions under consideration here. In particular, we explicitly give a sequence of coordinate transforms $\Phi_\varkappa$ which allows us to rewrite (1.3) as an integral over a unit cube $[0,1]^{2d}$:

$$I = \int_{S^{(1)}} \int_{S^{(2)}} F(x, y, y - x)\, dy dx = \int_{t \in [0,1]^{2d}} \sum_{\varkappa=1}^{K} (F \circ \Phi_\varkappa)(t) J_{\Phi_\varkappa}(t)\, dt. \tag{3.1}$$

More importantly, $\Phi_\varkappa$ isolates the singularity in the univariate direction t_1. Then, I in (3.1) is approximated numerically on the unit cube by a suitable quadrature rule with nodes $\{t_\mu\}_{\mu=1}^n$ and weights $\{\eta_\mu\}_{\mu=1}^n$ (a specific one-dimensional quadrature rule must be applied in the "singular" direction t_1), leading to the quadrature rule in the physical domain

$$Q_N = \sum_{\mu=1}^{n} \sum_{\varkappa=1}^{K} F \circ \Phi_\varkappa(t_\mu) J_{\Phi_\varkappa}(t_\mu) \eta_\mu \equiv \sum_{\mu=1}^{n} \sum_{\varkappa=1}^{K} F(x_{\mu\varkappa}, y_{\mu\varkappa}, z_{\mu\varkappa}) w_{\mu\varkappa}, \tag{3.2}$$

with the total number of nodes $N = nK$. The transformed nodes and weights are given in terms of the backward transform

$$(x_{\mu\varkappa}, y_{\mu\varkappa}, z_{\mu\varkappa}) := \Phi_\varkappa(t_\mu), \qquad w_{\mu\varkappa} := J_{\Phi_\varkappa}(t_\mu)\eta_\mu. \tag{3.3}$$

Enumeration with the single index $(\mu, \kappa) \to \lambda$ gives the desired quadrature rule (1.5). Hence, to obtain a quadrature on the physical domain $S^{(1)} \times S^{(2)}$, one needs to evaluate $\Phi_\varkappa(t)$ and $J_{\Phi_\varkappa}(t)$ for any $t \in [0,1]^{2d}$. Explicit evaluation of $\Phi_\varkappa$ and $J_{\Phi_\varkappa}$ is the focus of this section. To this end it will be convenient to split the evaluation into eight steps, which we discuss next.

Step 1: Transform $(x, y) \in S^{(1)} \times S^{(2)}$ to $(u, v) \in S_d \times S_d$. Suppose that $S^{(j)}$ are given by their vertices $v^{(j,0)}, \dots, v^{(j,d)}$ such that $v^{(1,j)} = v^{(2,j)}$ for $j = 0, \dots, k$ and $v^{(1,j)} \neq v^{(2,j)}$ for $j = k+1, \dots, d$. We agree that values $k \in \{-1, 0, 1, \dots, d\}$ are allowed. Then the case $k = -1$ represents two disjoint simplices, and $k = -1, 0, 1, \dots d$ represents the dimension of $S^{(1)} \cap S^{(2)}$ (with the convention that the dimension of the empty set equals -1).

From now on we agree that all vectors in $\mathbb{R}^d$ are given by the *row vectors* of their components. Consider two $d \times d$ transformation matrices

$$A^{(j)} := \begin{pmatrix} v^{(j,1)} - v^{(j,0)} \\ \dots \\ v^{(j,d)} - v^{(j,0)} \end{pmatrix}, \quad j = 1, 2.$$

They allow us to parametrize $x \in S^{(1)}, y \in S^{(2)}$ by $u, v \in S_d$ via the affine transform

$$x = v^{(1,0)} + uA^{(1)}, \qquad y = v^{(2,0)} + vA^{(2)}. \tag{3.4}$$

In the case of nontrivial intersection ($0 \le k \le d$) we observe that $v^{(2,0)} = v^{(1,0)}$ and the first k rows of $A^{(1)}$ and $A^{(2)}$ coincide:

$$A^{(j)} = \begin{pmatrix} B \\ B^{(j)} \end{pmatrix}, \quad B := \begin{pmatrix} v^{(j,1)} - v^{(j,0)} \\ \dots \\ v^{(j,k)} - v^{(j,0)} \end{pmatrix}, \quad B^{(j)} := \begin{pmatrix} v^{(j,k+1)} - v^{(j,0)} \\ \dots \\ v^{(j,d)} - v^{(j,0)} \end{pmatrix},$$

where $B \in \mathbb{R}^{k \times d}$ and $B^{(j)} \in \mathbb{R}^{(d-k) \times d}$. Let $\hat{u} := (u_1, \dots, u_k)$, $\check{u} := (u_{k+1}, \dots, u_d)$, and similarly for v; then for $\hat{z} := \hat{v} - \hat{u}$ and

$$z = y - x = \hat{z}B + \check{v}B^{(2)} - \check{u}B^{(1)} \tag{3.5}$$

there holds

$$I = \int_{u \in S_d} \int_{v \in S_d} G(u, v, \hat{v} - \hat{u})\, dv\, du \qquad \text{with} \tag{3.6}$$

$$G(u, v, \hat{z}) := \tilde{J} \cdot F\left(v^{(1,0)} + uA^{(1)}, v^{(2,0)} + vA^{(2)}, \hat{z}B + \check{v}B^{(2)} - \check{u}B^{(1)}\right), \tag{3.7}$$

$$\tilde{J} = \left|\det A^{(1)} \det A^{(2)}\right|.$$

The integrand G is singular if $(\check{u}, \check{v}, \hat{z}) = 0$; cf. [3, (3.11)] and part (i) of the proof of Theorem 4.1 below.

In the case $k = 0$ we adopt the convention $\check{u} := u$, $\check{v} := v$, and $\hat{u}, \hat{v}, \hat{z}$ do not appear in the integrand functions. There holds $A^{(j)} \equiv B^{(j)}$, and the integral (3.6) takes the form

$$I = \int_{u \in S_d} \int_{v \in S_d} G(u, v)\, dv\, du \qquad \text{with} \tag{3.8}$$

$$G(u, v) := \tilde{J} \cdot F\left(v^{(1,0)} + uA^{(1)}, v^{(2,0)} + vA^{(2)}, vA^{(2)} - uA^{(1)}\right). \tag{3.9}$$

In the case of disjoint simplices ($k = -1$) we have $\check{u} := u$, $\check{v} := v$, and

$$z = y - x = v^{(2,0)} - v^{(1,0)} + vA^{(2)} - uA^{(1)}. \tag{3.10}$$

In this case (3.8) also holds with the integrand

$$G(u, v) := \tilde{J} \cdot F\big(v^{(1,0)} + uA^{(1)}, v^{(2,0)} + vA^{(2)}, v^{(2,0)} - v^{(1,0)} + vA^{(2)} - uA^{(1)}\big). \tag{3.11}$$

Step 2 for $\boldsymbol{k = -1}$: Transform $\boldsymbol{(u, v) \in S_d \times S_d}$ to $\boldsymbol{(u, v) \in [0, 1]^{2d}}$. In case $k = -1$ the resulting integrand G in (3.11) is Gevrey-δ regular (or analytic if $\delta = 1$) in $S_d \times S_d$. We parametrize S_d by $[0, 1]^d$ as in (2.12) and obtain

$$I = \int_{(\bar{u},\bar{v})\in[0,1]^{2d}} G(\chi(\bar{u}), \chi(\bar{v}))\bar{u}_1^{d-1} \dots \bar{u}_{d-1}\bar{v}_1^{d-1} \dots \bar{v}_{d-1}\, d\bar{v}\, d\bar{u}. \tag{3.12}$$

According to [3, Proposition 3.3], the tensor product Gauss–Legendre quadrature rule achieves an exponential rate of convergence of the type (1.6) with $\gamma = 1/(2d\delta)$ for such integrands. In Theorem 5.4 below we prove that the Gauss–Jacobi quadrature rule absorbing monomial weights in (3.12) converges asymptotically at the same rate as the Gauss–Legendre quadrature rule.

The remaining coordinate transformations in Steps 2–8 are relevant only in the case $0 \le k \le d$.

Step 2: Transform $\boldsymbol{(u, v) \in S_d \times S_d}$ to $\boldsymbol{(\check{u}, \check{v}, \tilde{v}, \tilde{u}) \in S_{d-k} \times S_{d-k} \times S_k \times S_k}$. If $k \ge 1$, the intersection $S^{(1)} \cap S^{(2)}$ has a positive dimension k. In this case we will transform the integration over the intersection in Steps 2–6. If $k = 0$, the simplex S_k degenerates. In this case we say that S_0 is zero-dimensional. Similarly, we say that $\tilde{u} \in S_0$ is a zero-dimensional variable. We will use this terminology throughout the paper.

In the case $k = 0$ we can skip Steps 2–6 and go directly to Step 7 below because the intersection $S^{(1)} \cap S^{(2)}$ degenerates to a point. According to (2.5) we have

$$S_d = \{(\sigma_{\check{u}}\tilde{u}, \check{u}) \mid \tilde{u} \in S_k, \check{u} \in S_{d-k}\}$$

and similarly for v; thus it follows that

$$I = \int_{\check{u}\in S_{d-k}} \int_{\check{v}\in S_{d-k}} \int_{\tilde{v}\in S_k} \int_{\tilde{u}\in S_k} H(\check{u}, \check{v}, \tilde{v}, \tilde{u})\, d\tilde{u}\, d\tilde{v}\, d\check{v}\, d\check{u} \tag{3.13}$$

(cf. (2.6)), where

$$H(\check{u}, \check{v}, \tilde{v}, \tilde{u}) := G\left(\sigma_{\check{u}}\tilde{u}, \check{u}, \sigma_{\check{v}}\tilde{v}, \check{v}, \sigma_{\check{v}}\tilde{v} - \sigma_{\check{u}}\tilde{u}\right) \sigma_{\check{u}}^k \sigma_{\check{v}}^k. \tag{3.14}$$

The integrand H is singular at $(\check{u}, \check{v}, \tilde{v} - \tilde{u}) = 0$; see [3, Lemma 4.12] and part (ii) of the proof of Theorem 4.1.

Accurate float point evaluation of $\hat{z} = \sigma_{\check{v}}\tilde{v} - \sigma_{\check{u}}\tilde{u}$ is important for preventing subtractive cancellation of digits; cf. [3, Remark 3.7]. In particular, evaluation of $\hat{z}$ in the form

$$\hat{z} = \sigma_{\check{v}}\tilde{z} + \tilde{u}\sum_{i=1}^{d-k}(\check{u}_i - \check{v}_i), \tag{3.15}$$

where $\tilde{z} = \tilde{v} - \tilde{u}$ (see Step 3), helps to avoid subtractive cancellation.

This evaluation is unfortunately not possible if Ω_{op} is a piecewise smooth manifold in a higher dimensional space. A possible solution in this case is to use an asymptotic expansion of the integral kernel. We do not elaborate on the details and instead refer the reader to [7, Chapter 7]. In particular, we refer the reader to [7, section 7.2] for the change of coordinates in pseudohomogeneous kernels and to [7, section 8.5] for surface potentials on a boundary manifold.

We mention that S_k is zero-dimensional if $k=0$. In this case $\check{u}\equiv u$, $\check{v}\equiv v$, and (3.13) formally hold in view of (3.8), and (3.9) is reduced to

$$I=\int_{\check{u}\in S_d}\int_{\check{v}\in S_d} H(\check{u},\check{v})\,d\check{v}\,d\check{u} \quad \text{with} \quad H(\check{u},\check{v}):=G(u,v).$$

Step 3: Transform $(\tilde{v},\tilde{u})\in S_k\times S_k$ to $\{(\tilde{z},\tilde{u})\mid \tilde{z}\in A_k, \tilde{u}\in E_k(\tilde{z})\}$. Let $\tilde{z}:=\tilde{v}-\tilde{u}\in A_k$ where $A_k:=S_k-S_k=\{y-x\mid x,y\in S_k\}$. Then for a fixed value of the outer integration variable $\tilde{z}\in A_k$ we need the inner integration variable $\tilde{u}$ such that $\tilde{u}\in S_k$ and $\tilde{v}=\tilde{u}+\tilde{z}\in S_k$. In other words, for a fixed $\tilde{z}\in A_k$, the variable $\tilde{u}$ belongs to a $\tilde{z}$-dependent domain $E_k(\tilde{z}):=S_k\cap(S_k-\tilde{z})$. This construction gives a new representation for I which is equivalent to (3.13):

$$I=\int_{\check{u}\in S_{d-k}}\int_{\check{v}\in S_{d-k}}\int_{\tilde{z}\in A_k}\int_{\tilde{u}\in E_k(\tilde{z})} H(\check{u},\check{v},\tilde{z}+\tilde{u},\tilde{u})\,d\tilde{u}\,d\tilde{z}\,d\check{v}\,d\check{u}. \tag{3.16}$$

Step 4: Reflections. Due to [3, Lemma 3.6] we have with $M=\{1,\dots,k\}$ the following decomposition: $A_k=\bigcup_{N\subset M}A_{N,M\setminus N}$, where

$$\begin{aligned} A_{N^-,N^+} &:= \left\{z\in A_k \mid z_{N^-}\le 0, z_{N^+}\ge 0\right\} \\ &= \left\{z \mid z_{N^-}\in -S_{\#N^-}, z_{N^+}\in S_{\#N^+}\right\}. \end{aligned} \tag{3.17}$$

Every subdomain A_{N^-,N^+} admits further decomposition into a disjoint union of two pyramids $A_{N,M\setminus N}=A^+_{N,M\setminus N}\cup A^-_{N,M\setminus N}$, where

$$\begin{aligned} A^+_{N^-,N^+} &:= \left\{z\in A_{N^-,N^+} \mid \textstyle\sum_j z_j\ge 0\right\} \\ &= \left\{sz \mid z_{N^-}\in -S_{\#N^-};\ z_{N^+}\in B_{\#N^+};\ s\in[0,1]\right\}, \end{aligned} \tag{3.18}$$

$$\begin{aligned} A^-_{N^-,N^+} &:= \left\{z\in A_{N^-,N^+} \mid \textstyle\sum_j z_j\le 0\right\} \\ &= \left\{sz \mid z_{N^-}\in -B_{\#N^-};\ z_{N^+}\in S_{\#N^+};\ s\in[0,1]\right\}. \end{aligned} \tag{3.19}$$

Define

$$E^{\pm}_{N^-,N^+}(\tilde{z}):=-\tilde{z}^{(N^-)}+\left(1\mp\sum_j(\tilde{z}_{N^\pm})_j\right)S_d. \tag{3.20}$$

Note that $E^+_{N^-,N^+}(\tilde{z})$ takes the following explicit form:

$$E^+_{N^-,N^+}(\tilde{z})=-\tilde{z}^{(N^-)}+\sigma_{\tilde{z}_{N^+}}S_d. \tag{3.21}$$

According to [3, Lemma 3.6] we have

$$\tilde{z}\in A^{\pm}_{N^-,N^+} \quad \text{yielding} \quad E_k(\tilde{z})=E^{\pm}_{N^-,N^+}(\tilde{z}). \tag{3.22}$$

Collecting the terms, we obtain a new representation for the integral I in (3.16):
(3.23)

$$I = \sum_{N\subset M} \sum_{\sigma\in\{-,+\}} \int_{\check{u}\in S_{d-k}} \int_{\check{v}\in S_{d-k}} \int_{\tilde{z}\in A^{\sigma}_{N,M\setminus N}} \int_{\tilde{u}\in E^{\sigma}_{N,M\setminus N}(\tilde{z})} H(\check{u},\check{v},\tilde{z}+\tilde{u},\tilde{u})\, d\tilde{u}\, d\tilde{z}\, d\check{v}\, d\check{u}.$$

The double sum runs over $2^{k+1}-2$ many terms, because the subdomains $A^{-}_{\{\},M}$ and $A^{+}_{M,\{\}}$ are trivial. Definitions (3.18), (3.19), and (3.20) directly yield

$$A^{-}_{N^-,N^+} = -A^{+}_{N^+,N^-} \qquad \text{and} \qquad E^{-}_{N^-,N^+}(-\tilde{z}) = \tilde{z} + E^{+}_{N^+,N^-}(\tilde{z}).$$

Interchanging the integration and summation over σ, we obtain from (3.23)

$$I = \sum_{N\subsetneq M} \int_{\check{u}\in S_{d-k}} \int_{\check{v}\in S_{d-k}} \int_{\tilde{z}\in A^{+}_{N,M\setminus N}} \int_{\tilde{u}\in E^{+}_{N,M\setminus N}(\tilde{z})} f(\check{u},\check{v},\tilde{z},\tilde{u})\, d\tilde{u}\, d\tilde{z}\, d\check{v}\, d\check{u} \tag{3.24}$$

with

$$f(\check{u},\check{v},\tilde{z},\tilde{u}) := H(\check{u},\check{v},\tilde{z}+\tilde{u},\tilde{u}) + H(\check{u},\check{v},\tilde{u},\tilde{z}+\tilde{u}). \tag{3.25}$$

Note that f is singular at $(\check{u},\check{v},\tilde{z})=0$ and is regular with respect to $\tilde{u}$.

Step 5: Permutations. Now we group the subsets N with $\#N = j$ together for each $j = 0,\dots,k-1$. For every proper subset $N \subsetneq M$ of cardinality j and any vector $v\in\mathbb{R}^k$ we define a permutation operator P_N satisfying

$$w = P_N v \qquad \Leftrightarrow \qquad w_N = (v_1,\dots,v_j) \quad \text{and} \quad w_{M\setminus N} = (v_{j+1},\dots,v_k). \tag{3.26}$$

Then for $N_j := \{1,\dots,j\}$, $R_j := \{j+1,\dots,k\}$ there holds for any $N\subsetneq M$

$$\{(\tilde{z},\tilde{u}) \,|\, \tilde{z}\in A^{+}_{N,M\setminus N}, \tilde{u}\in E^{+}_{N,M\setminus N}(\tilde{z})\} = \{(P_N\tilde{z}, P_N\tilde{u}) \,|\, \tilde{z}\in A^{+}_{N_j,R_j}, \tilde{u}\in E^{+}_{N_j,R_j}(\tilde{z})\}.$$

In other words, all domains $A^{+}_{N,M\setminus N}$ and $E^{+}_{N,M\setminus N}(\tilde{z})$ with the same cardinality of the index set N can be treated as images of the reference domains $A^{+}_{N_j,R_j}$ and $E^{+}_{N_j,R_j}(\tilde{z})$ under a suitable coordinate permutation. As there exist only k different pairs of reference domains, this allows us to rewrite (3.24) in the following equivalent form, reducing the number of distinct domains of integration. For $k=0,\dots,d$ the integral I takes the form

$$\begin{aligned} I &= \sum_{j=0}^{\max(k-1,0)} I_j, \qquad \text{where} \\ I_j &:= \int_{\check{u}\in S_{d-k}} \int_{\check{v}\in S_{d-k}} \int_{\tilde{z}\in A^{+}_{N_j,R_j}} \int_{\tilde{u}\in E^{+}_{N_j,R_j}(\tilde{z})} g_j(\check{u},\check{v},\tilde{z},\tilde{u})\, d\tilde{u}\, d\tilde{z}\, d\check{v}\, d\check{u} \end{aligned} \tag{3.27}$$

and

$$g_j(\check{u},\check{v},\tilde{z},\tilde{u}) := \sum_{\substack{N\subset M,\\ \#N=j}} f(\check{u},\check{v},P_N\tilde{z},P_N\tilde{u}). \tag{3.28}$$

We remark that (3.27) and (3.28) formally hold also if $k=0$. In this case we necessarily have $j=0$ and

$$I = I_0 := \int_{\check{u}\in S_d} \int_{\check{v}\in S_d} g_0(\check{u},\check{v})\, d\check{v}\, d\check{u} \quad \text{with} \quad g_0(\check{u},\check{v}) := f(\check{u},\check{v}). \tag{3.29}$$

All functions g_j in (3.28), (3.29) have singular support $(\check{u},\check{v},\tilde{z})=0$ because $\tilde{z}=0$ iff $P_N\tilde{z}=0$.

Step 6: Transform $\tilde{u}\in E^+_{N_j,R_j}(\tilde{z})$ to $\bar{u}\in[0,1]^d$. Using representation (3.21) of $E^+_{N_j,R_j}(\tilde{z})$ and parametrization (2.12), we introduce

(3.30)
$$h_j(\check{u},\check{v},\tilde{z}):=\int_{\tilde{u}\in E^+_{N_j,R_j}(\tilde{z})} g_j(\check{u},\check{v},\tilde{z},\tilde{u})\,d\tilde{u}=\int_{\tilde{u}\in S_k} g_j(\check{u},\check{v},\tilde{z},-\tilde{z}^{(N_j)}+\sigma_{\tilde{z}_{R_j}}\tilde{u})\,\sigma^k_{\tilde{z}_{R_j}}\,d\tilde{u}$$

$$=\int_{\bar{u}\in[0,1]^k} g_j(\check{u},\check{v},\tilde{z},-\tilde{z}^{(N_j)}+\sigma_{\tilde{z}_{R_j}}\chi(\bar{u}))\,\sigma^k_{\tilde{z}_{R_j}}\,\bar{u}_1^{k-1}\dots\bar{u}_{k-1}\,d\tilde{u} \tag{3.31}$$

and thus

$$I_j=\int_{\check{u}\in S_{d-k}}\int_{\check{v}\in S_{d-k}}\int_{\tilde{z}\in A^+_{N_j,R_j}} h_j(\check{u},\check{v},\tilde{z})\,d\tilde{z}\,d\check{v}\,d\check{u}. \tag{3.32}$$

Note that in this equation some of the sets $S_{d-k}, A^+_{N_j,R_j}$ may be zero-dimensional. In this case the corresponding integration in (3.32) should be omitted. For instance, $A^+_{N_j,R_j}$ and $E^+_{N_j,R_j}(\tilde{z})$ are zero-dimensional for $k=0$. In this case $j=0$ and there formally hold

$$I_0=\int_{\check{u}\in S_d}\int_{\check{v}\in S_d} h_0(\check{u},\check{v})\,d\check{v}\,d\check{u},\qquad h_0(\check{u},\check{v})=h_0(\check{u},\check{v},\tilde{z})=g_0(\check{u},\check{v}).$$

The simplex S_{d-k} is zero-dimensional for $k=d$, and we have

$$I_j=\int_{\tilde{z}\in A^+_{N_j,R_j}} h_j(\tilde{z})\,d\tilde{z},\qquad h_j(\tilde{z})=h_j(\check{u},\check{v},\tilde{z}).$$

All integrands h_j are singular at the origin $(\check{u},\check{v},\tilde{z})=0$.

Step 7: Transform $(\check{u},\check{v},\tilde{z})\in S_{d-k}\times S_{d-k}\times A^+_{N_j,R_j}$ to $(s_1,a,s_2,b,p,s_3,q)\in[0,1]^{2d-k}$. Recall parametrizations (2.8), (2.9), and (3.18). Their combination allows us to use the following equivalent parametrizations for $\check{u},\check{v}\in S_{d-k}$ and $\tilde{z}\in A^+_{N_j,R_j}$:

$$\check{u}\in S_{d-k}=\{(\sigma_a s_1, s_1 a)\,|\,s_1\in[0,1], a\in S_{d-k-1}\}, \tag{3.33}$$

$$\check{v}\in S_{d-k}=\{(\sigma_b s_2, s_2 b)\,|\,s_2\in[0,1], b\in S_{d-k-1}\}, \tag{3.34}$$

$$\tilde{z}\in A^+_{N_j,R_j}=\{(-s_3 p,\sigma_q s_3, s_3 q)\,|\,p\in S_j, s_3\in[0,1], q\in S_{k-j-1}\}. \tag{3.35}$$

Depending on particular values of j,k,d certain subdomains in (3.33)–(3.35) may be zero-dimensional. This gives the following cases.

Case a: $1\le k\le d-1$. We get for $s=(s_1,s_2,s_3)$

$$I_j=\int_{s\in[0,1]^3} T_j(s)(s_1 s_2)^{d-k-1}s_3^{k-1}\,ds_3\,ds_2\,ds_1, \tag{3.36}$$

where for $h_j\equiv h_j\left((\sigma_a s_1, s_1 a),(\sigma_b s_2, s_2 b),(-s_3 p,\sigma_q s_3, s_3 q)\right)$ we set

$$T_j(s):=\int_{a\in S_{d-k-1}}\int_{b\in S_{d-k-1}}\int_{p\in S_j}\int_{q\in S_{k-j-1}} h_j\,dq\,dp\,db\,da. \tag{3.37}$$

Depending on j,k,d we have the following structure:

1. If $2 \le k \le d-2$, $1 \le j \le k-2$, then none of the subdomains in (3.37) is zero-dimensional.
2. If $0 = j \le k-2$, then S_j is zero-dimensional and $(-s_3 p, \sigma_q s_3, s_3 q) = (\sigma_q s_3, s_3 q)$.
3. If $1 \le j = k-1$, then S_{k-j-1} is zero-dimensional and $(-s_3 p, \sigma_q s_3, s_3 q) = (-s_3 p)$.
4. If $k = 1$, then both subdomains S_j and S_{k-j-1} are zero-dimensional and $(-s_3 p, \sigma_q s_3, s_3 q) = (s_3)$. Note that $s_3^{k-1} = 1$ in (3.36) in this case.
5. If $k = d-1$, then S_{d-k-1} is zero-dimensional and $((\sigma_a s_1, s_1 a), (\sigma_b s_2, s_2 b)) = (s_1, s_2)$. Note that $(s_1 s_2)^{d-k-1} = 1$ in (3.36) in this case.

We use the parametrization of a simplex by a cube from (2.11) and (2.12), $a = \chi(\bar{a})$, and similarly for b, p, q. Then $T_j(s)$ from (3.36) reads

(3.38)
$$T_j(s) = \int_{\bar{a}\in[0,1]^{d-k-1}} \int_{\bar{b}\in[0,1]^{d-k-1}} \int_{\bar{p}\in[0,1]^{j}} \int_{\bar{q}\in[0,1]^{k-j-1}} h_j J_\chi(\bar{a}) J_\chi(\bar{b}) J_\chi(\bar{p}) J_\chi(\bar{q})\, d\bar{q}\, d\bar{p}\, d\bar{b}\, d\bar{a}$$

with the function

$$h_j \equiv h_j\left((\sigma_{\chi(\bar{a})} s_1, s_1\chi(\bar{a})), (\sigma_\chi(\bar{b}) s_2, s_2\chi(\bar{b})), (-s_3\chi(\bar{p}), \sigma_{\chi(\bar{q})} s_3, s_3\chi(\bar{q}))\right)$$

and monomial weights J_χ defined in (2.15).

Case b: $k = 0$. In this case $A^+_{N_j,R_j}$ is zero-dimensional and we get for $s = (s_1, s_2)$

(3.39)
$$I_0 = \int_{s\in[0,1]^2} T_0(s)(s_1 s_2)^{d-1}\, ds_2\, ds_1, \qquad \text{with}$$

(3.40)
$$T_0(s) := \int_{\bar{a}\in[0,1]^{d-1}} \int_{\bar{b}\in[0,1]^{d-1}} h_0\left((\sigma_{\chi(\bar{a})} s_1, s_1\chi(\bar{a})), (\sigma_{\chi(\bar{b})} s_2, s_2\chi(\bar{b}))\right) \cdot J_\chi(\bar{a}) J_\chi(\bar{b})\, d\bar{b}\, d\bar{a}.$$

Case c: $k = d$. Then $S_{d-k} \times S_{d-k}$ is zero-dimensional and we get for $s = s_3$

$$I_j = \int_{s_3\in[0,1]} T_j(s_3) s_3^{d-1}\, ds_3, \tag{3.41}$$

where

$$T_j(s_3) = \int_{\bar{p}\in[0,1]^{j}} \int_{\bar{q}\in[0,1]^{k-j-1}} h_j\left(-s_3\chi(\bar{p}), \sigma_{\chi(\bar{q})} s_3, s_3\chi(\bar{q})\right) J_\chi(\bar{p}) J_\chi(\bar{q})\, d\bar{q}\, d\bar{p}. \tag{3.42}$$

Depending on values of j, k, d, cases a.1–a.4 are valid here. We remark that all integrands T_j in cases **a**, **b**, and **c** are singular iff $s = 0$.

Step 8: Integration over s in a cube.

Case a: $1 \le k \le d-1$. Here I_j in (3.36) reads

$$\begin{aligned} I_j = \int_{r\in[0,1]^3} &\big(T_j(r_1, r_1r_2, r_1r_3) + T_j(r_1r_2, r_1, r_1r_3)\big) r_1^{2d-k-1} r_2^{d-k-1} r_3^{k-1} \\ &+ \left(T_j(r_1r_2, r_1r_3, r_1)\right) r_1^{2d-k-1} (r_2r_3)^{d-k-1}\, dr_3\, dr_2\, dr_1. \end{aligned} \tag{3.43}$$

Case b: $k = 0$. Then I_j in (3.36) takes the form

$$I_j = \int_{r\in[0,1]^2} \left(T_j(r_1, r_1r_2) + T_j(r_1r_2, r_1)\right) r_1^{2d-1} r_2^{d-1}\, dr_2\, dr_1. \tag{3.44}$$

Case c: $k = d$. In this case no transform is needed, and we get

$$I_j = \int_{r_1\in[0,1]} T_j(r_1) r_1^{d-1}\, dr_1. \tag{3.45}$$

Note that the integrands in all three cases are singular only in $r_1 = 0$ and regular in the remaining variables.

Remark 2. In summary, we have rewritten the integral (1.3) as

$$I = \sum_{j=0}^{\min(k-1,0)} I_j, \qquad I_j = \int_{t\in[0,1]^{2d}} \sum_{\kappa=1}^{K_j} (F\circ\Phi_{\kappa j})(t) J_{\Phi_{\kappa j}}(t)\, dt. \tag{3.46}$$

Enumeration with a single summation index $(\kappa, j) \to \varkappa$ brings (3.46) into the desired form (3.1). Hence, the quadrature strategy described in the beginning of the present section can be applied. Here, t stands for the collection of all integration variables in the unit cube $[0,1]^{2d}$ after the transformations in Steps 1–8, i.e., $2d$ variables $r, \bar{a}, \bar{b}, \bar{p}, \bar{q}, \bar{u}$. We identify $t_1 = r_1$ as the singular variable.

Remark 3. We observe that the Jacobians can be factored, i.e.,

$$J_{\Phi_{\kappa j}}(t) = t_1^{2d-k-1} J^{\text{mon}}_{\Phi_{\kappa j}}(t_2,\ldots,t_{2d}) J^{\text{rem}}_{\Phi_{\kappa j}}(t), \tag{3.47}$$

where $J^{\text{mon}}_{\Phi_{\kappa j}}$ is a product of monomials and $J^{\text{rem}}_{\Phi_{\kappa j}}$ is a polynomial remainder. Precisely,

$$J^{\text{mon}}_{\Phi_{\kappa j}} = \begin{cases} J_\chi(\bar{u})J_\chi(\bar{v}), & k=-1,\\ r_2^{d-1} J_\chi(\bar{a})J_\chi(\bar{b}), & k=0,\\ \left\{\begin{array}{c} r_2^{d-k-1} r_3^{k-1} J_\chi(\bar{a})J_\chi(\bar{b})J_\chi(\bar{p})J_\chi(\bar{q})J_\chi(\bar{u}) \\ \text{and} \\ (r_2 r_3)^{d-k-1} J_\chi(\bar{a})J_\chi(\bar{b})J_\chi(\bar{p})J_\chi(\bar{q})J_\chi(\bar{u}) \end{array}\right\}, & 1\le k\le d,\\ J_\chi(\bar{p})J_\chi(\bar{q})J_\chi(\bar{u}), & k=d, \end{cases} \tag{3.48}$$

where, according to (2.13),

$$J_\chi : \begin{cases} [0,1]^m & \to \quad \mathbb{R},\\ \quad t & \mapsto \quad t_1^{m-1}\ldots t_{m-1}. \end{cases}$$

Note the following:

- The singular coordinate t_1 is not contained in $J^{\text{mon}}_{\Phi_{\kappa j}}$.
- In the case $k > 0$, the dimension of $\bar{a}, \bar{b}, \bar{p}, \bar{q}$, and hence the exact form of the Jacobians in (3.48) depends on the parameter j.
- The splitting (3.47) follows solely from the explicit form of the coordinate transforms in Steps 1–8 and not from the particular assumptions on the integrand. Hence it is valid, e.g., for the general class of admissible integrands satisfying (1.4).

Having the splitting (3.47), the monomial part $J_{\Phi_{\kappa j}}$ can be incorporated into the quadrature weights in terms of the tensor product Gauss–Jacobi quadrature. Suppose $\{(t^{GJ}_{\mu\kappa j}, w^{GJ}_{\mu\kappa j})\}_{\mu=1}^n$ is the corresponding quadrature rule, i.e.,

$$\int_{t\in[0,1]^{2d}} F_1(t) J^{\text{mon}}_{\Phi_{\kappa j}}(t_2,\ldots,t_{2d})\, dt \approx \sum_\mu F_1(t^{GJ}_{\mu\kappa j}) w^{GJ}_{\mu\kappa j}$$

for some sufficiently smooth F_1. Then

$$I \approx Q_N^{GJ} := \sum_{\mu=1}^{n} \sum_{j=0}^{\min(k-1,0)} \sum_{\kappa=1}^{K_j} F(x_{\mu\kappa j}, y_{\mu\kappa j}, z_{\mu\kappa j}) w_{\mu\kappa j},$$

where $N = n(K_0 + \cdots + K_{\min(k-1,0)})$ and

$$(x_{\mu\kappa j}, y_{\mu\kappa j}, z_{\mu\kappa j}) = \Phi_{\kappa j}(t_{\mu\kappa j}^{GJ}), \qquad w_{\mu\kappa j} = t_1^{2d-k-1} J_{\Phi_{\kappa j}}^{\mathrm{rem}}(t) w_{\mu\kappa j}^{GJ}|_{t=t_{\mu\kappa j}^{GJ}}.$$

Note that $J_{\Phi_{\kappa j}}^{\mathrm{mon}} = t^{\beta_{(\kappa j)}}$ for a suitable multi-index $\beta_{(\kappa j)} = (0, \beta_2, \ldots, \beta_{2d})$ with integer entries. In Theorems 5.3 and 5.4 we prove exponential convergence for this type of quadrature rule.

Remark 4. In the case of volume or surface layer potentials for second order elliptic operators there are two possible cases:

1. The singularity of $F(x, y, z)$ is of the type $\|z\|^\alpha$ with integer α. More precisely, the integrand satisfies [10, section 5.1.3]
(3.49)
$$F(x, y, z) = \|z\|^\alpha \tilde{F}(x, y, z), \qquad \tilde{F}(x, y, z) = \hat{F}(x, y, \|z\|, z/\|z\|),$$
$\hat{F}(x, y, r, \theta)$ analytic in $x \in S^{(1)}$, $y \in S^{(2)}$, $r \in [0, R]$, $\theta \in \{z \in \mathbb{R}^d \mid \|z\| = 1\}$.
After applying the transformations in Steps 1–8, the integrands will become analytic in *all* variables; see [3, Remark 4.3]. In this case the variable t_1 can be treated the same as the remaining variables. In this case the full tensor product Gauss–Legendre quadrature rule achieves exponential convergence (1.6) with $\gamma = 1/(2d\delta)$ for *all* $k = -1, 0, \ldots, d$ instead of $\gamma = 1/(2d\delta + 1)$ if a composite Gauss–Legendre quadrature rule [11] is used in t_1 [3, Theorem 4.5].
2. For elliptic PDEs in two dimensions the fundamental solution has a logarithmic singularity. Therefore, single layer potentials and volume potentials have a logarithmic singularity, and $F(x, y, z)$ has a singularity of type $\|z\|^{\alpha_0} \log \|z\|$ with integer α_0. In this case (1.4) is satisfied with $\alpha = \alpha_0 - \varepsilon$ for any $\varepsilon > 0$.

We prove in Theorem 5.4 below that an exponential convergence with $\gamma = 1/(2d\delta)$ can be also achieved for integrands of the type (3.49) and noninteger $\alpha > k - 2d$ with the aid of a suitable Gauss–Jacobi quadrature rule applied in the t_1-direction.

4. Explicit structure of the transformed singularity F satisfying (1.7).

The main result of this section is the proof of the following theorem.

THEOREM 4.1. *Suppose $k = \dim(S^{(1)} \cap S^{(2)}) \geq 0$ and the integrand F in (1.3) has the structure*

$$F(x, y, z) = \|z\|^\alpha \tilde{F}(x, y, z), \tag{4.1}$$

where $\alpha > k - 2d$ and $\tilde{F} \in G^\delta(S^{(1)} \times S^{(2)} \times (S^{(2)} - S^{(1)}))$ for some $\delta \geq 1$. Then after the coordinate transforms from section 3, the integral I in (1.3) takes the form

$$I = \int_{[0,1]^{2d}} t_1^{\alpha+2d-k-1} \mathcal{R}(t)\, dt \tag{4.2}$$

with some $\mathcal{R} \in G^\delta([0, 1]^{2d})$.

Proof. It suffices to prove that under the coordinate transforms in section 3 the function

$$\frac{\|y(t) - x(t)\|^\alpha}{t_1^\alpha}$$

is analytic in $t \in [0,1]^{2d}$. Then the assertion follows by Propositions A.1 and A.2 and the fact that the coordinate transformations in section 3 are polynomial and hence analytic, i.e., belong to $G^1([0,1]^{2d})$. The regularizing effect of the coordinate transforms in section 3 is due to the Jacobian determinant t_1^{2d-k-1}, appearing in (3.43)–(3.45). The transformations are rather complex, and we split

$$\frac{\|y-x\|^\alpha}{t_1^\alpha} = \frac{\|y-x\|^\alpha}{\|(\check{u},\check{v},\hat{v}-\hat{u})\|^\alpha}\frac{\|(\check{u},\check{v},\hat{v}-\hat{u})\|^\alpha}{\|(\check{u},\check{v},\tilde{z})\|^\alpha}\frac{\|(\check{u},\check{v},\tilde{z})\|^\alpha}{\|s\|^\alpha}\frac{\|s\|^\alpha}{t_1^\alpha} =: \mathcal{A}_1\mathcal{A}_2\mathcal{A}_3\mathcal{A}_4$$

for the sake of convenience. We show analyticity of all four fractions in the right-hand side separately. We follow here the strategy in [10, Chapter 5], [12, 11] restricted to the special case $d = 2$. We represent each $\mathcal{A}_i$ in the form $\mathcal{A}_i = \|\omega\|^\alpha$ for some suitable analytic (in fact, polynomial) ω and show that ω has no real roots in the integration domain. This implies analyticity of $\mathcal{A}_i$.

(i) We introduce polar coordinates (r,θ) satisfying

$$\zeta := (\check{u},\check{v},\hat{v}-\hat{u}) = r\theta, \qquad r = \|\zeta\|, \quad \theta = \frac{\zeta}{\|\zeta\|} = (\theta^{(1)},\theta^{(2)},\theta^{(3)}).$$

The aim is to show that $\mathcal{A}_1 = \mathcal{A}_1(\theta)$ is analytic in the polar coordinates. Here the subvector $\theta^{(3)}$ is empty if $k = 0$ and $\theta^{(1)}$, $\theta^{(2)}$ are empty if $k = d$. Recalling transformation (3.5), we find

$$y - x = r\omega(\theta), \qquad \omega(\theta) = \begin{cases} & \theta^{(2)}B^{(2)} - \theta^{(1)}B^{(1)}, & k=0,\\ \theta^{(3)}B & + \quad \theta^{(2)}B^{(2)} - \theta^{(1)}B^{(1)}, & 0<k<d,\\ \theta^{(3)}B, & & k=d.\end{cases} \tag{4.3}$$

Note that $\omega(\theta)$ is a linear map and hence is analytic. According to [3, (3.9)] there exists $c_1 > 0$ such that $\|y-x\| \geq c_1\|\zeta\| = c_1 r$, yielding

$$\|\omega(\theta)\| = \frac{\|y-x\|}{r} \geq c_1 > 0.$$

Then, $\omega(\theta)$ is never zero for θ corresponding to $(\hat{u},\check{u}),(\hat{v},\check{v}) \in S_d$, and hence $\mathcal{A}_1 = \frac{\|y-x\|^\alpha}{r^\alpha} = \|\omega(\theta)\|^\alpha$ is analytic. This covers the coordinate transformation in Step 1.

(ii) If $k = 0$, we have $\mathcal{A}_2 = 1$. Suppose $0 < k \leq d$. Let us redefine the polar coordinates

$$\zeta := (\check{u},\check{v},\tilde{z}) = r\theta, \qquad r = \|\zeta\|, \quad \theta = \frac{\zeta}{\|\zeta\|} = (\theta^{(1)},\theta^{(2)},\theta^{(3)})$$

and prove that $\mathcal{A}_2$ is analytic as a function of $r,\theta,\tilde{u}$. Recalling transformations in Step 2 of section 3, in particular relation (3.15), we find $(\check{u},\check{v},\hat{v}-\hat{u}) = r\omega(r,\theta,\tilde{u})$, where

$$\omega(r,\theta,\tilde{u}) = \begin{cases} \left(\theta^{(1)},\theta^{(2)},\theta^{(3)}\sigma_{(r\theta^{(2)})} + \tilde{u}\sum_{j=1}^{d-k}(\theta^{(1)}-\theta^{(2)})\right), & 0<k<d,\\ \theta^{(3)}, & k=d.\end{cases}$$

Lemma 4.12 from [3] provides the estimate

$$\|\omega(r,\theta,\tilde{u})\| = \frac{\|(\check{u},\check{v},\hat{v}-\hat{u})\|}{r} \geq c_2 > 0$$

uniformly in the domain of integration. Therefore, the polynomial $\omega(r,\theta,\tilde{u})$ is nonzero if $(\tilde{u},\check{u}),(\tilde{v},\check{v}) \in S_k \times S_{d-k}$; thus $\mathcal{A}_2 = \frac{\|(\check{u},\check{v},\hat{v}-\hat{u})\|^\alpha}{r^\alpha} = \|\omega(r,\theta,\tilde{u})\|^\alpha$ is analytic. This result covers the transformations in Step 2. In Steps 3–5 only domain partition happens, and the transformation in Step 6 does not influence the singularity. This gives the desired result for transformations in Steps 2–6.

(iii) Let us consider the function $\mathcal{A}_3$. For

$$s = \begin{cases} (s_1, s_2), & k = 0, \\ (s_1, s_2, s_3), & 0 < k < d, \\ s_3, & k = d, \end{cases}$$

we introduce polar coordinates via the relation

$$s = r\theta, \qquad r = \|s\|, \quad \theta = \frac{s}{\|s\|} = \left\{ \begin{array}{cc} (\theta_1, \theta_2), & k = 0 \\ (\theta_1, \theta_2, \theta_3), & 0 < k < d \\ \theta_3, & k = d \end{array} \right\}$$

and show that $\mathcal{A}_3 = \mathcal{A}_3(\theta)$ is an analytic function is polar coordinates. Combining all the transformations in Step 7, we obtain

$$(\check{u}, \check{v}, \tilde{z}) = r\omega(\theta, a, b, p, q), \qquad \omega(\theta, a, b, p, q) = (\sigma_a\theta_1, \theta_1 a, \sigma_b\theta_2, \theta_2 b, -\theta_3 p, \sigma_q\theta_3, \theta_3 q),$$

where some components of ω may vanish depending on the values of j, k, d; cf. Step 7. For the $\|\cdot\|_1$-norm we have

$$\|\omega\|_1 \geq \|\theta\|_1 \min\{\|(\sigma_a, a)\|_1, \|(\sigma_b, b)\|_1, \|(\sigma_q, q)\|_1\} \geq \|\theta\|_1$$

because $\|(\sigma_a, a)\|_1 = |1 - \sum a_j| + \sum |a_j| \geq 1$. Since in a finite dimensional space all norms are equivalent, we have $\|\omega\| \geq c_3(d)\|\theta\| = c_3(d) > 0$ uniformly in the domain of integration, and hence ω is nonzero. Hence $\mathcal{A}_3 = \frac{\|(\check{u},\check{v},\tilde{z})\|^\alpha}{r^\alpha} = \|\omega\|^\alpha$ is analytic. This covers the coordinate transformations in Step 7.

(iv) Finally, we prove that $\mathcal{A}_4$ is analytic. In Step 8 the variables s are transformed to variables r according to (3.43)–(3.45), and r_1 is identified with t_1. In all three cases we have $s = t_1\omega(r)$ with

$$\omega(r) = \begin{cases} (1, r_2), & k = 0, \\ (1, r_2, r_3), & 0 < k < d, \\ 1, & k = d, \end{cases}$$

up to a permutation. Therefore, $\|\omega(r)\| \geq 1$, yielding that $\mathcal{A}_4 = \frac{\|s\|^\alpha}{t_1^\alpha} = \|\omega(r)\|^\alpha$ is an analytic function of r. The proof is complete. $\square$

5. Convergence of Gauss–Jacobi quadrature rules. In this section we give convergence results for tensor product quadratures involving one-dimensional Gauss–Jacobi rules.

5.1. Convergence of the Gauss–Jacobi quadrature for Gevrey-δ integrands on an interval. Suppose $\alpha, \beta > -1$ are fixed parameters, and consider a continuous function g on an open interval (a,b) such that $\int_a^b |g(x)|(b-x)^\alpha(x-a)^\beta\,dx < \infty$. We approximate the integral

$$I^{[a,b],(\alpha,\beta)}[f] := \int_a^b g(x)(b-x)^\alpha(x-a)^\beta\,dx$$

by the Gauss–Jacobi quadrature rule:

$$Q_n^{[a,b],(\alpha,\beta)}[f] := \sum_{i=1}^{n} g(x_i) w_i.$$

The Gauss–Jacobi quadrature rule is exact for polynomials of degree up to $2n-1$; cf. [8, Chapter 7.3].

THEOREM 5.1. *Let $n \in \mathbb{N}$ and $k \in \{2, 3, \dots, 2n-1\}$. Then for $g \in C^k([a,b])$*

$$\begin{aligned} &\left|I^{[a,b],(\alpha,\beta)}[g] - Q_n^{[a,b],(\alpha,\beta)}[g]\right| \\ &\qquad \le \left(\frac{b-a}{2}\right)^{\alpha+\beta+k+1} \frac{\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)} \frac{2^{\alpha+\beta+3}\|g^{(k)}\|_\infty}{(k-1)(2n-k)^{k-1}}. \end{aligned} \tag{5.1}$$

Proof. We first consider $[a,b] = [-1,1]$. $Q_n^{[-1,1],(\alpha,\beta)}$ is exact of degree $2n-1$; hence for an arbitrary polynomial ψ of degree up to $2n-1$

$$\begin{aligned} \left|I^{[-1,1],(\alpha,\beta)}[g] - Q_n^{[-1,1],(\alpha,\beta)}[g]\right| &\le \left|I^{[-1,1],(\alpha,\beta)}[g-\psi]\right| + \left|Q_n^{[-1,1],(\alpha,\beta)}[g-\psi]\right| \\ &\le 2I^{[-1,1],(\alpha,\beta)}[1]\|g-\psi\|_\infty \end{aligned}$$

and $I^{[-1,1],(\alpha,\beta)}[1] = 2^{\alpha+\beta+1}\Gamma(\alpha+1)\Gamma(\beta+1)/\Gamma(\alpha+\beta+2) < \infty$, since $\alpha, \beta > -1$. We choose a particular $\psi := T_{2n-1}[g]$ as the Chebyshev approximation of degree $2n-1$ to g. According to [14, Theorem 4.3] this yields the bound

$$\|g-\psi\|_\infty \le \frac{2\|g^{(k)}(x)/\sqrt{1-x^2}\|_1}{\pi(k-1)(2n-k)^{k-1}} \le \frac{2\|g^{(k)}\|_\infty}{(k-1)(2n-k)^{k-1}}.$$

An affine transformation to $[a,b]$ yields the assertion. ∎

THEOREM 5.2. *Assume that $g \in G^\delta([a,b])$ with $\delta \ge 1$ and constants A_0, A_1 in (1.2). Let $\rho := A_1(b-a)/2$. Let*

$$r_* := \begin{cases} 2\log\left[\rho^{-1} + \sqrt{1+\rho^{-2}}\right], & \delta = 1, \\ \delta\rho^{-1/\delta}, & \delta > 1. \end{cases}$$

Then for any $r < r_*$ there exists $C > 0$ depending only on $r, \rho, \alpha, \beta,$ and δ such that for all $n \in \mathbb{N}$

$$|I^{[a,b],(\alpha,\beta)}[g] - Q_n^{[a,b],(\alpha,\beta)}[g]| \le A_0(b-a)^{\alpha+\beta+1} C \exp(-rn^{1/\delta}). \tag{5.2}$$

Proof. The proof is analogous to [3, Theorem 2.3]. In the case $\delta = 1$ the only difference is the factor $(\frac{b-a}{2})^{\alpha+\beta+1}$ appearing while scaling $[a,b]$ to $[-1,1]$ in [3, (2.4)]. In the case $\delta > 1$ the expression $\frac{32}{15}\frac{b-a}{2}$ in [3, (2.5)] changes to $(\frac{b-a}{2})^{\alpha+\beta+1}2^{\alpha+\beta+3} \cdot \frac{\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)}$ according to Theorem 5.1. ∎

5.2. Tensor product quadrature on $[0,1]^d$. The following theorems follow directly from Theorem 5.2, two theorems from [3], [3, Theorems 2.5 and 2.7], and the tensor product argument in [3, Proposition 2.8].

THEOREM 5.3. *Suppose $d \in \mathbb{N}$, $\delta \geq 1$, and $\alpha > -1$, and assume that $g \in G^{\delta,\alpha}_{\{1\}}([0,1]^d)$. Let $Q_{n,m}$ be the constant or variable order composite Gauss–Legendre quadrature rule on $[0,1]$ with m subintervals and n nodes in the largest subinterval, $m \sim n^{1/\delta}$; cf.* [3, Definition 2.4]. *Let $\beta = (0, \beta_2, \dots, \beta_d)$ be a multi-index satisfying $\beta > -1$ and $Q_n^{\beta_i} = Q_n^{[0,1],(0,\beta_i)}$ be a family of Gauss–Jacobi quadratures with n nodes. Then there exist $C, r, r' > 0$ independent of d such that for all $n \in \mathbb{N}$*

$$\left| \int_{[0,1]^d} g(t) t^\beta \, dt - Q_{n,m} \otimes Q_n^{\beta_2} \otimes \cdots \otimes Q_n^{\beta_d}[g] \right| \leq C \exp(-r n^{1/\delta}) \leq C \exp(-r' N^{1/(d\delta+1)}), \tag{5.3}$$

where $N = \mathcal{O}(n^{d+\delta^{-1}})$ is the total number of quadrature nodes.

THEOREM 5.4. *Suppose $d \in \mathbb{N}$ and $\delta \geq 1$, and assume that $g \in G^\delta([0,1]^d)$. Let $\beta = (\beta_1, \beta_2, \dots, \beta_d)$ be a multi-index satisfying $\beta > -1$, and let $Q_n^{\beta_i} = Q_n^{[0,1],(0,\beta_i)}$ be a family of Gauss–Jacobi quadratures with n nodes. Then there exist $C, r, r' > 0$ independent of d such that for all $n \in \mathbb{N}$*

$$\left| \int_{[0,1]^d} g(t) t^\beta \, dt - Q_n^{\beta_1} \otimes Q_n^{\beta_2} \otimes \cdots \otimes Q_n^{\beta_d}[g] \right| \leq C \exp(-r n^{1/\delta}) \leq C \exp(-r' N^{1/(d\delta)}), \tag{5.4}$$

where $N = \mathcal{O}(n^d)$ is the total number of quadrature nodes.

6. Numerical examples.

In this section we give convergence results for the suggested $2d$-dimensional quadratures involving one-dimensional Gauss–Jacobi quadrature rules and compare them to the hp-quadratures from [3].

6.1. Comparison of composite Gauss–Legendre and Gauss–Jacobi rules for Gevrey-δ integrands with singularity in one dimension.

In this section we compare performance of the composite Gauss–Legendre quadrature and the Gauss–Jacobi quadrature for a Gevrey-δ integrand with an algebraic singularity on an interval. Let us consider a function

$$f_{\alpha,p}(x) = (1-x)^\alpha g_p(x), \qquad g_p(x) = \begin{cases} \exp(-x^{-p}), & 0 < x \leq 1, \\ 0, & -1 \leq x \leq 0. \end{cases} \tag{6.1}$$

The function $f_{\alpha,p}$ has an integrable singularity at 1 if $\alpha > -1$, and is not analytic in any neighborhood of 0. Precisely, $g_p \in G^\delta([-1,1])$ iff $\delta \geq 1 + 1/p$; cf. [3]. According to Theorem 5.4, we expect the convergence rate of order $\mathcal{O}(\exp(-r' N^{1/\delta}))$ for the Gauss–Jacobi rule with the weight $(\alpha, 0)$. According to [3], we expect the convergence of order $\mathcal{O}(\exp(-r' N^{1/(2\delta)}))$ for the composite Gauss–Legendre rule. Convergence results for $p = 2$ and $\alpha = 1/\pi - 1$ given in Figure 6.1 show the sharpness of these estimates. We observe a clear advantage of the Gauss–Jacobi quadrature rule for integration of this type of singularity if the exponent α is known. The classical Gauss–Legendre quadrature rule converges slowly, because the integrand $f_{\alpha,p}$ has a singularity; see, e.g., [5].

6.2. Performance of Gauss–Jacobi quadrature rules for $2d$-dimensional integrands.

We consider the integral (1.3) for two particular simplices $S^{(1)} := S_d$ and $S^{(2)} := ((y_1, \dots, y_k, -y_{k+1}, \dots, -y_d) \mid y \in S_d)$, where $k = 0, \dots, d$, i.e., the intersection $S^{(1)} \cap S^{(2)} = \{(\hat{x}, 0, \dots, 0) \mid \hat{x} \in S_k\}$ is of dimension k. For $k = -1$ we use $S^{(1)} := S_d$ and $S^{(2)} := S_d - (1, \dots, 1)$.

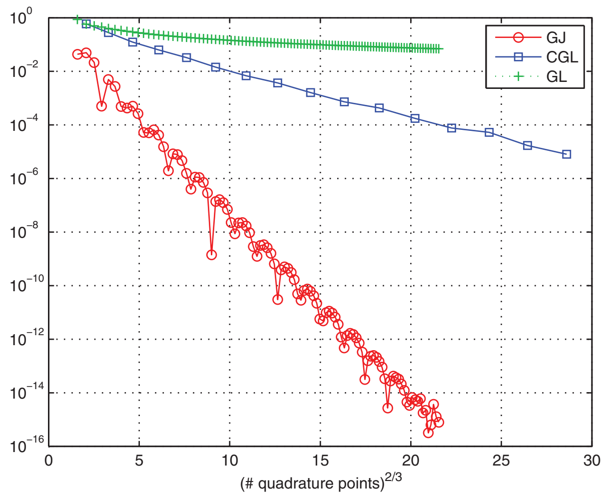

FIG. 6.1. *Comparison of Gauss–Jacobi, composite Gauss–Legendre, and Gauss–Legendre quadrature rules for the univariate Gevrey-δ integrand with an algebraic singularity from* (6.1).

We examine the performance of various transformed quadrature rules for the kernel

$$F(x, y, z) = \|z\|^{\alpha}, \qquad z = y - x, \quad \alpha = k - 2d + \beta \tag{6.2}$$

with $\beta > 0$; i.e., the exponent is larger by β than the critical exponent $k - 2d$, where $F(x, y, y - x) \notin L^1(S^{(1)} \times S^{(2)})$. Note that F satisfies assumptions (1.4) and (1.7). In this case, quadrature rules involving a suitable Gauss–Jacobi rule in the singular direction are expected to be more efficient than those using the general purpose composite Gauss–Legendre rule.

In our numerical experiments we used $\beta = 1/\pi$. We choose singularities very close to the nonintegrable case for *all* $k = 0, \ldots, d$ as a severe test for our algorithm. In applications for integral equations one has a fixed integrand $F(x, y, z) \sim \|z\|^{\alpha_*}$ with $\alpha_* > -d$ for all k, and $\beta = \beta_k := \alpha_* - (k - 2d) > d - k$.

As motivated in the beginning of section 3, any sufficiently accurate (e.g., exponentially converging) quadrature rule on the cube $t \in [0, 1]^{2d}$ for integrands with univariate algebraic singularity in t_1 and Gevrey-δ smooth in $(t_2, \ldots, t_{2d})$ yields an accurate (exponentially converging) quadrature rule in the physical domain by means of the transform in section 3. In what follows we compare three classes of tensor product quadrature rules corresponding to the following combination in the singular/regular directions on $[0, 1]^{2d}$:

1. composite Gauss–Legendre/Gauss–Legendre (CGL-GL),
2. Gauss–Jacobi/Gauss–Legendre (GJ-GL),
3. Gauss–Jacobi/Gauss–Jacobi (GJ-GJ).

In the tests we use the Gauss–Legendre and Gauss–Jacobi quadrature rules with n nodes in each direction. The parameters of the composite Gauss–Legendre quadrature rule are chosen as follows. Let $\tilde{n} = 2n$. We use a geometric mesh with ratio $\sigma = 0.1$ and $m = \tilde{n}$ subintervals, with $1, 2, \ldots, \tilde{n}$ Gauss–Legendre points on the subintervals; cf. [3] for the details.

Other combinations of quadrature rules are also possible. We refer the reader to [2] for more numerical examples, combining, e.g., Smolyak-type quadrature rules in the

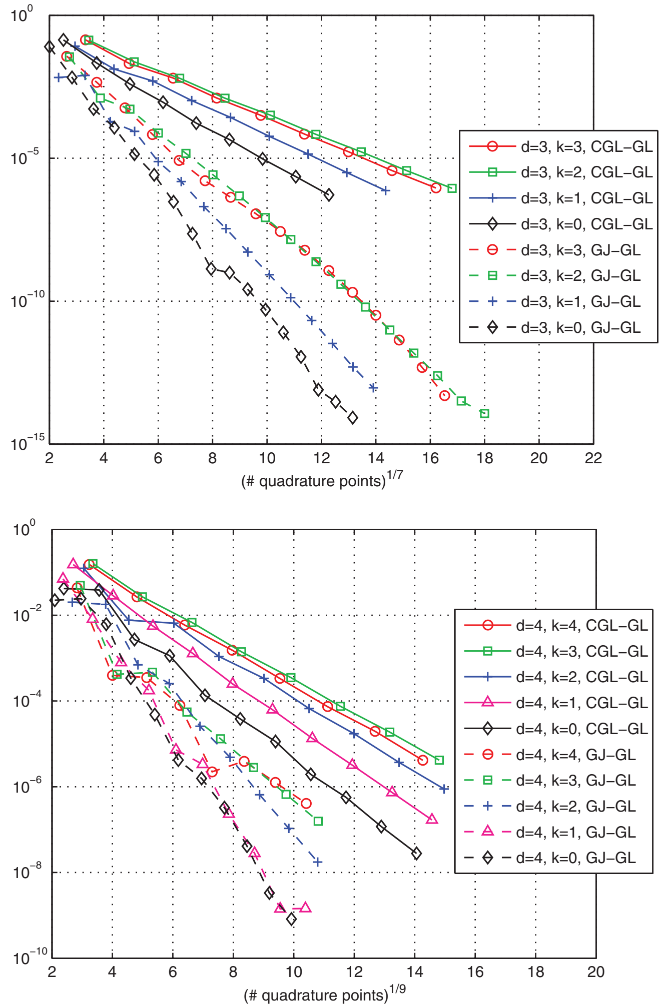

FIG. 6.2. *Comparison of CGL and GJ in the singular direction for* $F = \|y - x\|^{\alpha}$. *Relative error* $|I - Q_N|/|I|$ *for* $d = 3, 4$ *and* $k = 0, \dots, d$.

"regular" direction with the Gauss–Jacobi or composite Gauss–Legendre quadrature rule in the "singular" direction.

In the convergence plots we show on the vertical axis the relative error $|I - Q_N|/|I|$ in the logarithmic scale, and on the horizontal axis $N^{1/(2d+1)}$, where N is the total number of quadrature points (or function evaluations). This yields

$$N = \begin{cases} K \dfrac{\tilde{n}(\tilde{n}+1)}{2} n^{2d-1}, & 0 \le k \le d, \\ \qquad n^{2d}, & k = -1, \end{cases} \qquad K = \begin{cases} 2 & \text{for } k = 0, \\ 3(2^{k+1} - 2) & \text{for } 1 \le k \le d-1, \\ 2^{k+1} - 2 & \text{for } k = d. \end{cases}$$

The value of $K = K_0 + \cdots + K_{\min(k-1,0)}$ follows from the explicit form of the transformations in section 3

In Figure 6.2 we present the convergence history for the combinations CGL-GL and GJ-GL for $d = 3$ and 4 and the integrand (6.2). As the approximate integral value

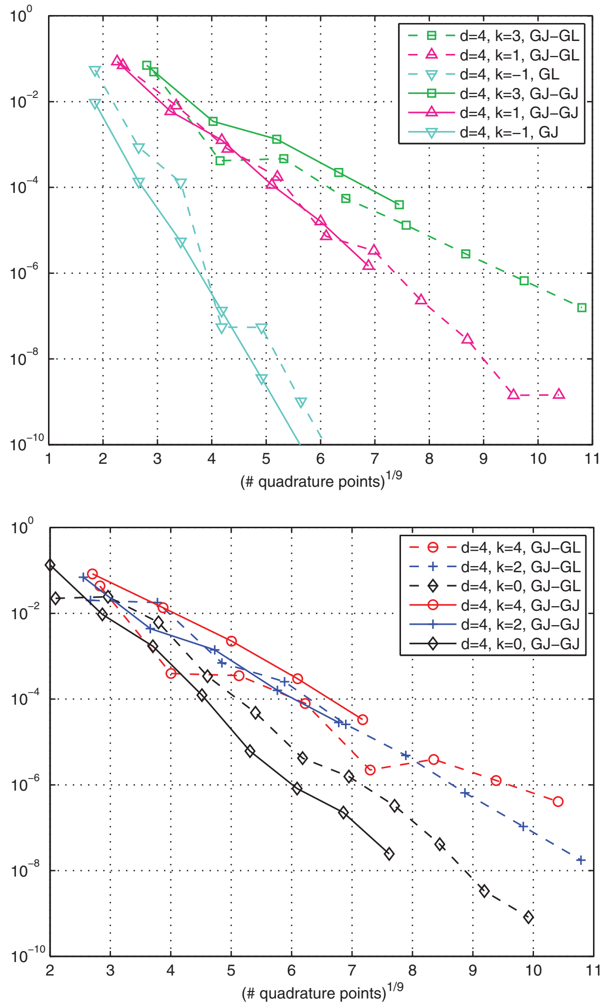

FIG. 6.3. *Comparison of GJ and GL in the regular direction for $F = \|y - x\|^{\alpha}$. Relative error $|I - Q_N|/|I|$ for $d = 4$ and $k = -1, \ldots, d$.*

we take the value of the GJ-GL quadrature on the finest discretization level. In both cases $d = 3$ and $d = 4$ we observe a strong improvement of several orders of magnitude if Gauss–Jacobi quadrature is used instead of the composite Gauss–Legendre rule in the singular direction.

In Figure 6.3 we compare the combinations GJ-GL and GJ-GJ. We observe that both quadrature rules provide almost the same quality of approximation: GJ-GJ is better for $k = -1, 0$, GJ-GL is better for $k = 3, 4$, and the error curves are very close for $k = 1, 2$. Taking into account that the implementation of the Gauss–Jacobi quadrature rule in the regular direction is somewhat more complex (e.g., the weights of the input quadrature depend on the parameter j; cf. Remark 3) and the simplices with many common vertices (i.e., for high k) cause the largest quadrature error, the combination GJ-GL is advisable for implementation for problems with kernels satisfying (1.7). In the case of more general singularities (1.4) the combination CGL-GL (not CGL-GJ) is advisable for the same reason.

Appendix. Here we prove two auxiliary results on regularity of the product and composition of Gevrey-δ functions.

PROPOSITION A.1. *Suppose $f \in G^{\delta_1}(\Omega)$ and $g \in G^{\delta_2}(\Omega)$ for some $\Omega \subseteq \mathbb{R}^m$ and $\delta_1, \delta_2 \geq 1$. Then the product $fg \in G^{\max\{\delta_1,\delta_2\}}(\Omega)$.*

Proof. By definition (1.2), there exist $A_0, A_1, B_0, B_1 > 0$ such that

$$|D^\nu f(x)| \leq A_0 A_1^{|\nu|}(\nu!)^{\delta_1}, \qquad |D^\nu g(x)| \leq B_0 B_1^{|\nu|}(\nu!)^{\delta_2} \qquad \forall \nu \in \mathbb{N}_0^m, \quad \forall x \in \Omega.$$

Then, by the m-dimensional product rule

$$\begin{aligned} |D^\nu fg| &= \left| \sum_{0\leq\beta\leq\nu} \begin{pmatrix} \nu \\ \beta \end{pmatrix} D^{\nu-\beta} f D^\beta g \right| \\ &\leq \sum_{0\leq\beta\leq\nu} \begin{pmatrix} \nu \\ \beta \end{pmatrix} A_0 A_1^{|\nu-\beta|}((\nu-\beta)!)^{\delta_1} B_0 B_1^{|\beta|}(\beta!)^{\delta_2} \\ &\leq A_0 B_0 (A_1 + B_1)^{|\nu|}(\nu!)^{\max\{\delta_1,\delta_2\}}, \end{aligned}$$

and hence $fg \in G^{\max\{\delta_1,\delta_2\}}(\Omega)$ by (1.2). $\square$

PROPOSITION A.2. *Assume that $\delta_1, \delta_2 \geq 1$ and $f \in G^{\delta_1}(\Omega_1)$, $g \in G^{\delta_2}(\Omega_2)$ for some $\Omega_2 \subseteq \mathbb{R}^{m_2}$ and* Range $g \subseteq \Omega_1 \subseteq \mathbb{R}^{m_1}$*. Then $f \circ g \in G^{\delta_1+\delta_2-1}(\Omega_2)$.*

Proof. We recall a multivariate version of the formula of Faà di Bruno [4], which represents the chain rule for composition of multivariate functions

$$D_x^\nu (f\circ g)(x) = \sum_{\ell=1}^{|\nu|} \sum_{\left(\substack{j_1,\dots,j_\ell \\ \beta_{(1)},\dots,\beta_{(\ell)}}\right) \in \mathcal{M}_{\nu,\ell}} \gamma^{|\nu|,m_2,\ell}_{j,\beta_{(1)},\dots,\beta_{(\ell)}} (D^l_{y_{j_1}\dots y_{j_\ell}} f(y)) \prod_{i=1}^{\ell} (D_x^{\beta_{(i)}} g_{j_i}(x)).$$

Here $\gamma^{|\nu|,m_2,\ell}_{j,\beta_{(1)},\dots,\beta_{(l)}}$ are positive integers, and the sum is taken over the set

(A.1)
$$\mathcal{M}_{\nu,\ell} := \left\{ \begin{pmatrix} j_1,\dots,j_\ell \\ \beta_{(1)},\dots,\beta_{(\ell)} \end{pmatrix} : \begin{array}{c} j_1,\dots,j_\ell \in \{1,\dots,m_1\} \qquad \text{and} \\ \beta_{(1)}+\cdots+\beta_{(\ell)} = \nu \ \wedge\ \beta_{(i)} \neq 0, i = 1,\dots,\ell \end{array} \right\}.$$

Note that $j_1,\dots,j_\ell$ are integers and $\beta_{(1)},\dots,\beta_{(\ell)}$ are multi-indices of the same length as ν, that is, m_2. We have

$$\begin{aligned} |D_x^\nu (f\circ g)(x)| &\leq \sum_{\ell=1}^{|\nu|} \sum_{\left(\substack{j_1,\dots,j_\ell \\ \beta_{(1)},\dots,\beta_{(\ell)}}\right) \in \mathcal{M}_{\nu,\ell}} \gamma^{|\nu|,m_2,\ell}_{j,\beta_{(1)},\dots,\beta_{(\ell)}} \left| D^l_{y_{j_1}\dots y_{j_\ell}} f(y)\right| \prod_{i=1}^{\ell} \left| D_x^{\beta_{(i)}} g_{j_i}(x)\right| \\ &\leq \sum_{\ell=1}^{|\nu|} \sum_{\left(\substack{j_1,\dots,j_\ell \\ \beta_{(1)},\dots,\beta_{(\ell)}}\right) \in \mathcal{M}_{\nu,\ell}} \gamma^{|\nu|,m_2,\ell}_{j,\beta_{(1)},\dots,\beta_{(\ell)}} A_0 A_1^\ell (\ell!)^{\delta_1} \prod_{i=1}^{\ell} B_0 B_1^{|\beta_{(i)}|}(\beta_{(i)}!)^{\delta_2}. \end{aligned}$$

From (A.1) we get $\sum_{i=1}^\ell |\beta_{(i)}| = |\nu|$ and $\prod_{i=1}^\ell (\beta_{(i)}!) \leq \nu!$; hence

$$\begin{aligned} |D_x^\nu (f\circ g)(x)| &\leq A_0 (A_1 B_0 B_1)^{|\nu|} \sum_{\ell=1}^{|\nu|} \sum_{\left(\substack{j_1,\dots,j_\ell \\ \beta_{(1)},\dots,\beta_{(\ell)}}\right) \in \mathcal{M}_{\nu,\ell}} \gamma^{|\nu|,m_2,\ell}_{j,\beta_{(1)},\dots,\beta_{(\ell)}} (\ell!)^{\delta_1} \prod_{i=1}^{\ell} (\beta_{(i)}!)^{\delta_2} \\ &\leq A_0 (A_1 B_0 B_1)^{|\nu|} (|\nu|!)^{\delta_1 - 1} (\nu!)^{\delta_2 - 1} \cdot \Theta \end{aligned}$$

with

$$\Theta = \sum_{\ell=1}^{|\nu|} \sum_{\binom{j_1,\dots,j_\ell}{\beta_{(1)},\dots,\beta_{(\ell)}} \in \mathcal{M}_{\nu,\ell}} \gamma^{|\nu|,m_2,\ell}_{j,\beta_{(1)},\dots,\beta_{(\ell)}} \ell! \prod_{i=1}^{\ell} (\beta_{(i)}!) \leq (m_1+1)^{|\nu|}|\nu|!,$$

where in the last step we applied the identity [4, (1.24)]. The multinomial theorem yields $|\nu|! \leq {m_2}^{|\nu|}\nu!$; therefore,

$$|D^\nu_x(f \circ g)(x)| \leq A_0(A_1B_0B_1{m_2}^{\delta_1})^{|\nu|}(\nu!)^{\delta_1+\delta_2-1}.$$

Hence $f \circ g \in G^{\delta_1+\delta_2-1}(\Omega_2)$ by (1.2). ∎

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