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EXPONENTIAL CONVERGENCE OF hp QUADRATURE FOR INTEGRAL OPERATORS WITH GEVREY KERNELS

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Abstract. Galerkin discretizations of integral equations in $\mathbb{R}^d$ require the evaluation of integrals $I = \int_{S^{(1)}} \int_{S^{(2)}} g(x,y)\mathrm{d}y\mathrm{d}x$ where $S^{(1)}, S^{(2)}$ are d-simplices and g has a singularity at $x = y$. We assume that g is Gevrey smooth for $x \neq y$ and satisfies bounds for the derivatives which allow algebraic singularities at $x = y$. This holds for kernel functions commonly occurring in integral equations. We construct a family of quadrature rules $\mathcal{Q}_N$ using N function evaluations of g which achieves exponential convergence $|I - \mathcal{Q}_N| \leq C \exp(-rN^\gamma)$ with constants $r, \gamma > 0$.

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Dedicated to Professor G.C. Hsiao on the occasion of his 75th anniversary.

1. Introduction

The numerical solution of singular integral equations

$$(\mathcal{K}u)(x) := c(x)u(x) + \int_{y\in\Omega} K(x,y)u(y)\mathrm{d}y = f(x) \quad \text{for all } x \in \Omega$$

for an unknown function u in a polyhedron or on its boundary $\Omega \subset \mathbb{R}^d$ is a basic problem in engineering. For integral operators $\mathcal{K}$ which are bounded, linear $\mathcal{K} : V \to V'$, the weak formulation of $\mathcal{K}u = f$ reads:

$$\text{find} \quad u \in V : \quad \langle v, \mathcal{K}u\rangle = \langle v, f\rangle \quad \forall v \in V.$$

Here, V denotes a suitable separable Hilbert space, V' its dual and $\langle\cdot,\cdot\rangle$ indicates the $V \times V'$ duality pairing. Problems of this type arise, for example, in the boundary reduction of linear, elliptic boundary value problems (*e.g.* [8,13,14,19]) or in Dirichlet forms for Markov Processes with jumps (*e.g.* [10]). Typically, the kernel function $K(x,y)$ is smooth for $x \neq y$, but possibly becomes strongly singular at $x = y$; in this case, integration with respect to $K(x,y)$ must be interpreted in a suitable sense (*e.g.* [15]).

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A common approximation method for these equations is Galerkin approximation: one restricts the above weak formulation to a space $V_h \subset V$ of piecewise polynomials on a mesh of simplices on Ω of width $h > 0$ spanned by a basis ϕ_i^h. Then one has to compute the elements of the stiffness matrix

$$A_{ij} = \int_{x\in\Omega}\int_{y\in\Omega} K(x,y)\phi_j^h(y)\phi_i^h(x)\mathrm{d}y\,\mathrm{d}x.$$

As the basis functions $\phi_j^h(x)$ are piecewise polynomials on simplices, this amounts to computing integrals of the type

$$I = \int_{x\in S^{(1)}}\int_{y\in S^{(2)}} K(x,y)v(x)w(y)\mathrm{d}y\,\mathrm{d}x = \int_{x\in S^{(1)}}\int_{y\in S^{(2)}} g(x,y)\mathrm{d}y\,\mathrm{d}x \tag{1.1}$$

where $S^{(1)}, S^{(2)}$ are *closed* simplices of the mesh and $v(x), w(y)$ are smooth (*e.g.* analytic) functions. If the original domain Ω is curved, or a manifold in a higher dimensional space (*e.g.* the boundary of a polyhedron in $\mathbb{R}^{d+1}$) one can use parameterizations and also has to compute integrals of the type (1.1) where the functions v, w may include parameterization mappings and Jacobians, but still are piecewise smooth functions on the mesh of simplices.

Note that the kernel function $K(x,y)$ may be nonintegrable (*i.e.* hypersingular or Cauchy singular) so that the integrand $g(x,y)$ in (1.1) is not in $L^1(S^{(1)}\times S^{(2)})$. The integral in (1.1) has therefore to be interpreted in a suitable sense: prior to numerical integration, methods for "regularizing" the integral A_{ij} resulting in an integrand $g(x,y)$ which belongs to $L^1(S^{(1)}\times S^{(2)})$ must be employed. There are, roughly speaking three basic approaches for regularization of integral equations with nonintegrable kernels: (i) exploit antisymmetry resp. parity of the most singular part of K: this implies a cancellation of the divergent parts of the integral and ensures the existence of the integrals in (1.1) in the sense of Cauchy principal value. Such antisymmetry properties of the kernel functions $K(x,y)$ in (1.1) appear in all integral equations obtained from boundary reduction of second order, strongly elliptic boundary value problems (*e.g.* [19], Chap. 5, and [8] or the exposition in [11]); (ii) formally perform integration by parts (*e.g.* [7,12,15] and, in particular [16], Chap. 5.6); or (iii) subtract terms from the functions ϕ_j and ϕ_i (*e.g.*, [17], Props. 4 and 5).

In the end one still obtains integrals of the type (1.1) where v, w are smooth, the function $g(x,y)$ is smooth for $x \neq y$ and singular for $x = y$, but $g \in L^1(S^{(1)}\times S^{(2)})$.

The main difficulty in implementing Galerkin methods for integral operators is the numerical approximation of the integrals (1.1) since the integrand is nonsmooth if $S^{(1)}\cap S^{(2)} \neq \{\}$.

In most applications the functions v, w are analytic and satisfy estimates of the type

$$|D^\nu v(x)| \le A_0 A_1^{|\nu|}\nu! \tag{1.2}$$

and the functions $K(x,y)$ and $g(x,y)$ can be written as $F(x,y,y-x)$ where F satisfies an estimate (*e.g.* [8], Chap. 9)

$$|D^\nu F(x,y,z)| \le A_0 A_1^{|\nu|}\nu!\,\|z\|^{\min(\alpha-|\nu_z|,0)}, \tag{1.3}$$

with the multiindices $\nu \in \mathbb{N}_0^{3d}$, $\nu_z := (\nu_{2d+1},\ldots,\nu_{3d})$ and $\alpha > k-2d$ if $S^{(1)}\cap S^{(2)}$ is k-dimensional with $k \in \{0,\ldots,d\}$ (note that this implies $g \in L^1(S^{(1)}\times S^{(2)})$). This is in fact the case for strongly elliptic boundary integral operators on boundaries of polyhedra (*e.g.* [8]) or, more generally, on piecewise smooth open or closed d-manifolds in $\mathbb{R}^{d+1}$.

The efficient accurate numerical evaluation of integrals (1.1) with integrand functions $g(x,y)$ which become singular at $x = y$ has attracted considerable attention over the years. In the (important) special case when the singularity order α in (1.3), (1.4) equal $\alpha = -1 > k-2d$ (as is the case *e.g.* for $K(x,y)$ given by the Coulomb potential), the singularity can be *removed completely* by a (degenerate) coordinate transformation (see [6] for the case $k = d = 2,3$ and [21] for $k = d = 2$). In these cases, Gaussian quadrature rules applied to the transformed integrands yield approximations which converge exponentially in terms of N, the number of quadrature nodes [21].

In boundary element methods on surfaces in $\mathbb{R}^3$ the singularity order α is always integer so that the above mentioned variable substitution described in [19], Chapter 5, can be applied. In integral equations which involve fundamental solutions of second order elliptic operators in $\mathbb{R}^2$, however, $F(x,y,z) \sim \log \|z\|$ as $z \to 0$ may occur. This case is not covered by the variable substitutions [6,21], but is contained in the assumptions (1.3) with $\alpha = -\varepsilon$ with arbitrary small $\varepsilon > 0$. In integral operators arising in integrodifferential generators of Markov processes with jumps such as Levy processes, noninteger α may occur (see, *e.g.*, [10,17]). In option pricing applications from finance, higher dimensions than $d = 3$ are also common (see, *e.g.*, [17]). Although in applications from engineering and the sciences, the kernel functions $K(x,y)$ are analytic in the sense that the estimate (1.3) holds, we shall present a quadrature error analysis for *Gevrey* regular kernel functions $K(x,y)$, of Gevrey class with index $\delta \geq 1$ which have been considered *e.g.* in [1,2]. These functions satisfy estimates (1.2), (1.3), however with the term $\nu!$ in (1.2), (1.3) replaced by $(\nu!)^\delta$:

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

Analytic functions correspond to the case $\delta = 1$. *E.g.*, the usual C^∞ cutoff functions are not analytic, but only in a Gevrey class with $\delta > 1$, see (6.2). This allows to treat more general problems involving Gevrey pseudodifferential operators investigated *e.g.* in [1], discretization methods of "generalized Finite Element type" where the basis functions ϕ_i^h of V_h are constructed with Gevrey-class cutoff functions or Gevrey partitions of unity.

It turns out in practice that the efficient approximation of the singular integrals is a difficult, because the convergence rates of standard (*e.g.* Gaussian) quadratures with N points deteriorate for integrand functions with a singularity, (*e.g.* [5] for an analysis of this).

Most methods in the literature rely on a very specific form of the kernel function $K(x,y)$ or geometry of $S^{(j)}$. Our proposed method has the advantage that it only uses pointwise evaluations of $g(x,y)$ (no antiderivatives needed), works for all integrands with (1.4) (which includes noninteger singularity orders and logarithmic singularities), and uses the same algorithm in all dimensions d and all possible cases how the two simplices $S^{(1)}, S^{(2)}$ may touch.

We will construct families of variable order, composite quadrature methods $\mathcal{Q}_N$ of the form $\mathcal{Q}_N = \sum_{j=1}^N w_j g(x_j, y_j)$ with N integrand evaluations such that, as $N \to \infty$, exponential convergence of the quadrature error is realized, *i.e.* we show for the integral I defined in (1.1) with integrand $g(x,y)$ satisfying (1.3) or (1.4) the asymptotic error estimate

$$|I - \mathcal{Q}_N| \leq C \exp(-rN^\gamma) \tag{1.5}$$

with constants $C, r, \gamma > 0$ depending on $A_0, A_1, \alpha, \delta, d$. Specifically, we prove for the quadrature of integrals (1.1) over the integration domains $S^{(1)} \times S^{(2)} \subset \mathbb{R}^{2d}$ with integrand function $g(x,y)$ satisfying (1.4) with $\delta > 1$ the error bound (1.5) with $\gamma = 1/(1+2d\delta)$. This allows, using estimates for the impact of the quadrature error upon the asymptotic accuracy of the Galerkin scheme as, *e.g.* in [19], Chapter 4.2, to obtain fully discrete h-version Boundary Element Methods on polygonal and polyhedral domains with analytic, possibly curved, sides, at a complexity which is, up to terms logarithmic in the number of degrees of freedom, not larger than the total number of degrees of freedom on the boundary.

In the context of hp-discretizations of strongly elliptic boundary integral equations which converge at an exponential rate in terms of the number of degrees of freedom (*e.g.* [23] and the references there), our quadrature methods imply *exponential convergence in terms of the total work* for all integral equations arising in engineering practice.

We assume that the mesh of simplices is shape regular, but not necessarily quasi uniform. This allows mesh refinement toward a point in the h-version and hp-version, and includes the meshes generated by standard adaptive methods. Anisotropic mesh refinement (*e.g.* with long and thin elements) is excluded, however.

In our case the kernel function only becomes singular for $y - x = 0$. In the numerical solution of Kolmogoroff equations for Markov processes with jumps arising, for example, in mathematical finance occur kernel functions

with anisotropic singularities which can also become singular for $y_j - x_j = 0$. This case is not treated here but the techniques developed herein can be suitably modified to deal with these cases (see, *e.g.* [25]).

We want to note that the same techniques also apply to other types of singular integrals, *e.g.* volume potentials applied to a function, or pointwise evaluation of a potential (*e.g.* in collocation methods).

The main idea of the quadrature in [20] is that 1D Gaussian quadrature converges exponentially if the integration interval is away from the singularity. If the integrand is singular at an endpoint, one can compensate for this by geometric refinement. Here we generalize the results of [20] in two directions: first, we establish exponential convergence rates for singular integrands with merely Gevrey regularity outside the compact support, and second, we address the treatment of double integrals (1.1) which arise in Galerkin discretizations of singular integral equations.

The paper is organized as follows: In Section 2 we prove convergence rates (1.5) with $\gamma = 1/(1+\delta)$ for Gevrey class G^δ functions with an endpoint singularity (functions in G^δ without endpoint singularity yield $\gamma = 1/\delta$) on the domain $[0,1]$ and also for tensor product quadrature on $[0,1]^d$. In the case of two simplices $S^{(1)}, S^{(2)}$ which do not touch one can obtain exponential convergence by simply using Gaussian integration in a suitable way. If the two simplices touch we give a sequence of transformations which isolate the singularity of the integrand in exactly one coordinate direction while preserving Gevrey regularity in the remaining $2d-1$ coordinates. We then apply a tensor product quadrature consisting of the composite Gauss quadrature from Section 2 in the singular coordinate direction and a $(2d-1)$-fold tensor product Gauss-Legendre quadrature in the remaining directions. The transformations and the resulting quadrature algorithm are described in Section 3. Section 4 proves the Gevrey regularity of the resulting transformed integrands and gives the main theorem about exponential convergence (1.5) of our quadrature algorithm. In Section 5 we consider an integral as in (1.1) with parallelotopes (images of cubes under affine maps) $C^{(1)}, C^{(2)}$ instead of the simplices $S^{(1)}, S^{(2)}$. In this case we obtain similar results. In Section 6 we give an example with $\delta > 1$ for an integral over $[0,1]$, and examples for integrals over $S^{(1)} \times S^{(2)} \subset \mathbb{R}^{2d}$ with $d = 2, 3$. The examples indicate that the asymptotic convergence estimates (1.5) are sharp.

1.1. **Definitions and notations**

Let $\mathbb{N}$ denote the set of positive integers and $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$. For a multiindex $\nu \in \mathbb{N}_0^d$ we use the standard notations $|\nu| = \sum_{i=1}^d \nu_i$, $\nu! = \prod_{i=1}^d \nu_i!$ and $D^\nu f(x) = \dfrac{\partial^{|\nu|}}{\partial x_1^{\nu_1} \dots \partial x_d^{\nu_d}} f(x)$ for a function $f\colon \Omega \to \mathbb{R}$ with $\Omega \subset \mathbb{R}^d$. For $x \in \mathbb{R}^d$ we let $\|x\| := \|x\|_2 = (\sum x_j^2)^{1/2}$. In integrals we write

$$\int_{x\in\Omega} f(x)\mathrm{d}x \qquad \text{for} \qquad \int_{x\in\Omega} f(x)\mathrm{d}x_1 \dots \mathrm{d}x_d.$$

Consider a subset $N = \{n_1, \dots, n_k\}$ of $\{1, \dots, d\}$ with $n_1 < \dots < n_k$. We will use the notation $x_N := (x_{n_1}, \dots, x_{n_k})$ and $\#N := k$. For $x \in \mathbb{R}^d$ we define $x^{(N)} \in \mathbb{R}^d$ 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.

We will now introduce the spaces G^δ of Gevrey functions and $G_N^{\delta,\alpha}$ of Gevrey functions with a singularity:

Definition 1.1. Let $D \subset \mathbb{R}^d$ be a closed bounded set and $\delta \geq 1$. A function $f\colon D \to \mathbb{R}$ is in $G^\delta(D)$ iff there exist $A_0, A_1 > 0$ so that

$$\forall x \in D, \forall \nu \in \mathbb{N}_0^d\colon \qquad |D^\nu f(x)| \leq A_0 A_1^{|\nu|} (\nu!)^\delta \tag{1.6}$$

(*i.e.*, the estimate holds *uniformly* on D).

Let $\alpha \in \mathbb{R}$, $N \subset \{1, \dots, d\}$. A function $f\colon D \to \mathbb{R}$ is in $G_N^{\delta,\alpha}(D)$ iff there exist $A_0, A_1 > 0$ so that

$$\forall x \in D \text{ with } x_N \neq 0, \forall \nu \in \mathbb{N}_0^d\colon \qquad |D^\nu f(x)| \leq A_0 A_1^{|\nu|} (\nu!)^\delta \|x_N\|^{\min\{0, \alpha - |\nu_N|\}}. \tag{1.7}$$

A function $f \in G_N^{\delta,\alpha}(D)$ may have a singularity at $x_N = 0$. *E.g.*, the function $f(x) = \|x_N\|^\alpha g(x) + h(x)$ with $\alpha \in \mathbb{R}$ and $g, h \in G^\delta(D)$ satisfies $f \in G_N^{\delta,\alpha}(D)$. In the case $N = \{1, \dots, d\}$ we will write $G^{\delta,\alpha}(D) := G_N^{\delta,\alpha}(D)$.

For sets $D_j \subset \mathbb{N}_0^d$ we write $D = D_1 \dot\cup \dots \dot\cup D_m$ if $D_i \cap D_j = \{\}$ for all i, j.

For functions $f, g \colon \Omega \to \mathbb{R}$ we will write $f \sim g$ if there exists $c, C > 0$ such that $cg(x) \le f(x) \le Cg(x)$ for all $x \in \Omega$.

Let $\Psi : \mathbb{R}^r \to \mathbb{R}^r$. We denote the absolute value of the Jacobian determinant of Ψ by

$$J_\Psi := |\det(D\Psi)|. \tag{1.8}$$

2. Quadrature of Gevrey functions with singularities on intervals

2.1. Introduction

We consider a function $g \in C^0((a,b)) \cap L^1((a,b))$ on an interval (a,b) and want to approximate the integral

$$\mathcal{I}g := \int_a^b g(x)\mathrm{d}x.$$

Definition 2.1. We denote by $Q_n g$ the Gauss-Legendre quadrature approximation of $\mathcal{I}g$ with n quadrature points for the interval $[a,b]$. If the interval is not clear from the context we will also write $Q_n^{[a,b]}g$ and $\mathcal{I}^{[a,b]}g$.

First assume that g is analytic on the closed interval $[a,b]$, *i.e.*, $g \in G^1([a,b])$. Then it is well known (*e.g.*, [24]) that there is exponential convergence: there exist $C, r > 0$ so that for all $n \in \mathbb{N}$

$$|\mathcal{I}g - Q_n g| \le C \exp(-rn).$$

We consider two generalizations where $g \in C^\infty((a,b))$ but may not be analytic on $[a,b]$:

(1) for $g \in G^\delta([a,b])$ with $\delta \ge 1$ we will obtain for n-point Gauss-Legendre quadrature Q_n on $(0,1)$ exponential convergence rates of the form $|\mathcal{I}g - Q_n g| \le C \exp(-rn^{1/\delta})$;

(2) for the interval $[a,b] = [0,1]$ assume that g has an algebraic singularity at 0 in the sense that $g \in G^{\delta,\alpha}([0,1])$ with $\delta \ge 1$, $\alpha > -1$. For $\delta = 1$ it is known that Gaussian quadrature converges in this case only with an algebraic rate $O(n^{-2(\alpha+1)})$, see, *e.g.*, [5]. In order to achieve exponential convergence we will use a geometric subdivision with $m = O(n^{1/\delta})$ subintervals and then use composite Gauss quadrature with n nodes on each subinterval. Then the quadrature error is bounded by $C \exp(-rN^{1/(1+\delta)})$ where N is the total number of quadrature points.

Therefore we always obtain an error bound $C \exp(-rN^\beta)$ with $\beta > 0$, but we pay for larger values of δ or the presence of a singularity with a smaller exponent β.

2.2. Convergence of Gauss-Legendre quadrature for Gevrey integrands

The classical error estimate for Gauss-Legendre quadrature uses the derivative $g^{(2n)}$. This formula can be used to prove exponential convergence of $Q_n g$ if g is analytic in a sufficiently large neighborhood of $[a,b]$. In order to prove exponential convergence for $g \in G^1([a,b])$ (g analytic in a neighborhood of $[a,b]$) and $g \in G^\delta([a,b])$ with $\delta > 1$ (where g may not be analytic) we need an estimate which allows to use lower order derivatives:

Lemma 2.2. *Let $n \in \mathbb{N}$ and $k \in \{2, 3, \dots, 2n-1\}$. Then we have for $g \in C^k([a,b])$*

$$|\mathcal{I}g - Q_n g| \le \frac{32}{15} \left(\frac{b-a}{2}\right)^{k+1} \frac{1}{(k-1)(2n-k)^{k-1}} \left\|g^{(k)}\right\|_\infty .$$

Proof. We first consider $[a,b]=[-1,1]$. Then Theorem 4.5 in [24] gives

$$|\mathcal{I}g - Q_n g| \le \frac{32}{15}\frac{1}{(k-1)(2n-k)^{k-1}}\left\|g^{(k)}\right\|_\infty$$

using $\left\|f(x)/(1-x^2)^{1/2}\right\|_1 \le \pi\,\|f\|_\infty$. A linear change of variables gives the result for general $[a,b]$. □

We now assume that $g \in G^\delta([a,b])$ with Gevrey index $\delta \ge 1$, and consider the convergence of Gauss quadrature $Q_n g$.

Theorem 2.3. *Assume that $g \in G^\delta([a,b])$ with $\delta \ge 1$ and constants A_0, A_1 in (1.6). Let $\rho := A_1(b-a)/2$. For $\delta = 1$ let*

$$r_* := 2\log\left[\rho^{-1} + \sqrt{1+\rho^{-2}}\right] \tag{2.1}$$

and for $\delta > 1$ let

$$r_* = \delta\rho^{-1/\delta}. \tag{2.2}$$

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

$$|\mathcal{I}g - Q_n g| \le A_0(b-a)C\exp\Big(-rn^{1/\delta}\Big). \tag{2.3}$$

Proof. **In the case** $\delta = 1$ we consider $\tilde g(z) := g(\frac{a+b}{2} + z\frac{b-a}{2})$ and see from its Taylor series that $\tilde g$ is analytic in $U := \{z \in \mathbb{C} \mid \operatorname{dist}(z,[-1,1]) < \rho^{-1}\}$ and $|\tilde g(z)| \le A_0/\left(1-\rho\operatorname{dist}(z,[-1,1])\right)$ for $z \in U$. For $s > 1$ let E_s denote the open ellipse $E_s := \{(z+z^{-1})/2 \mid z \in \mathbb{C},\ |z| < s\}$ with foci ± 1 where the sum of its semiaxes is s. The largest ellipse E_s contained in U is E_{s_*} with $s_* := \rho^{-1} + \sqrt{1+\rho^{-2}}$. By Theorem 4.5 in [24] we then obtain that for any $s \in (1, s_*)$

$$\left|\mathcal{I}^{[a,b]}g - Q_n^{[a,b]}g\right| = \frac{b-a}{2}\left|\mathcal{I}^{[-1,1]}\tilde g - Q_n^{[-1,1]}\tilde g\right| \le (b-a)M_s C_s s^{-2n} \tag{2.4}$$

where $M_s := \sup_{z\in E_s}|\tilde g(z)| \le A_0/(1-\rho(s-s^{-1})/2) < \infty$ as $(s_* - s_*^{-1})/2 = \rho^{-1}$. This gives (2.1), (2.3).

In the case $\delta > 1$ let $E_n := |\mathcal{I}g - Q_n g|$. Then Lemma 2.2, (1.6) and the Stirling estimate $k! \le 1.1(2\pi k)^{1/2}k^k\mathrm{e}^{-k}$ give for any $k \in \{2,3,\dots,2n-1\}$

$$\begin{aligned} E_n &\le \frac{32}{15}\left(\frac{b-a}{2}\right)^{k+1}\frac{1}{(k-1)(2n-k)^{k-1}}A_0A_1^k(k!)^\delta \\ &\le \left[A_0\frac{b-a}{2}\frac{32}{15}1.1^\delta(2\pi)^{\delta/2}\right]\left[A_1\frac{b-a}{2}\mathrm{e}^{-\delta}\right]^k\frac{k^{\delta/2}(2n-k)}{k-1}\frac{k^{\delta k}}{(2n-k)^k} = c_\delta\frac{k^{\delta/2}(2n-k)}{k-1}\left(\frac{\tilde\rho k^\delta}{2n-k}\right)^k \end{aligned} \tag{2.5}$$

where $\tilde\rho := A_1\frac{b-a}{2}\mathrm{e}^{-\delta} = \rho\mathrm{e}^{-\delta}$. We now want to choose k such that $f(k) := \left(\frac{\tilde\rho k^\delta}{2n-k}\right)^k$ is small. Let $\kappa = \mathrm{e}^{-1}(n/\tilde\rho)^{1/\delta}$ and $k = \lfloor\kappa\rfloor$. If $k \le n$ and $\kappa \ge 1$ we have

$$f(k) \le \left(\frac{\tilde\rho}{n}k^\delta\right)^k \le \left(\frac{\tilde\rho}{n}\kappa^\delta\right)^\kappa = \mathrm{e}^{-\delta\kappa}.$$

If $\kappa \ge n$ we let $k := n$. As $\kappa \ge n \iff n \le (\mathrm{e}^\delta\tilde\rho)^{-1/(\delta-1)}$ we obtain $f(k) = \tilde\rho^n n^{(\delta-1)n} \le \mathrm{e}^{-\delta n}$. Note that $\kappa < 2 \iff n < 2^\delta\mathrm{e}^\delta\tilde\rho$ occurs only for $n \le C_{\delta,\rho}$ so that we still have $f(k) \le c_{\delta,\rho}\mathrm{e}^{-\delta\kappa}$ for $n \in \mathbb{N}$.

Finally we note that the term $\frac{k^{\delta/2}(2n-k)}{k-1}$ in (2.5) grows at most algebraically in n and can therefore be absorbed in (2.3) by using $r < r_*$. □

2.3. Composite Gauss quadrature for singularity at endpoint of interval

We now consider the interval $[a,b]=[0,1]$ and an integrand $g(x)$ which may be singular at 0 in the sense that $g\in G^{\delta,\alpha}([0,1])$ with $\delta\geq 1$ and $\alpha>-1$. Note that $\alpha>-1$ implies $g\in L^1([0,1])$.

Let $m\in\mathbb{N}$ and $\sigma\in(0,1)$. We define the geometric subdivision $[0,1]=I_1\cup\ldots\cup I_m$ with

$$I_j:=[\sigma^j,\sigma^{j-1}]\quad\text{for } j=1,\ldots,m-1;\qquad I_m:=[0,\sigma^{m-1}]. \tag{2.6}$$

We then define two types of composite Gauss quadrature rules on this subdivision:

Definition 2.4. For $m,n\in\mathbb{N}$ and $\sigma\in(0,1)$ let I_j be given by (2.6). We define the *constant order composite Gauss rule*

$$Q_{n,m,\sigma}g:=\sum_{j=1}^{m}Q_n^{I_j}g. \tag{2.7}$$

For $\delta\geq 1$ we define the *variable order composite Gauss rule* by

$$n_j:=\left\lceil\frac{n(m+1-j)^\delta}{m^\delta}\right\rceil\quad\text{for } j=1,\ldots,m;\qquad Q_{n,m,\sigma,\delta}g:=\sum_{j=1}^{m}Q_{n_j}^{I_j}g. \tag{2.8}$$

We will write $Q_{n,m}$ for results which hold for both $Q_{n,m}=Q_{n,m,\sigma}$ and $Q_{n,m}=Q_{n,m,\sigma,\delta}$.

The constant order rule $Q_{n,m,\sigma}$ uses n Gauss points on each subinterval and has hence a total of $N=mn$ quadrature points. The variable order rule $Q_{n,m,\sigma,\delta}$ uses $n_1=n$ Gauss points on the rightmost interval I_1, and a decreasing number of Gauss points towards 0. The total number of quadrature points is $N=\sum_{j=1}^m n_j\approx nm/(\delta+1)$.

Theorem 2.5. *Assume that $g\in G^{\delta,\alpha}([0,1])$ with $\delta\geq 1$, $\alpha>-1$. Let $\sigma\in(0,1)$, $b>0$. Then the constant order composite rule $Q_{n,m,\sigma}$ with $m=\lceil bn^{1/\delta}\rceil$ has a total number of evaluation points $N=O(n^{1+\delta^{-1}})$ and there exist $C,r,r'>0$ such that for all $n\in\mathbb{N}$*

$$|\mathcal{I}g-Q_{n,m,\sigma}g|\leq C\exp(-r'n^{1/\delta})\leq C\exp(-rN^{1/(1+\delta)}). \tag{2.9}$$

Proof. Define $\hat\alpha:=\min\{\alpha,2\}$. Then $g\in G^{\delta,\alpha}\implies g\in G^{\delta,\hat\alpha}$. An interval $I_j=[\sigma^j,\sigma^{j-1}]$ with $j<m$ has length $\ell_j=\sigma^j(\sigma^{-1}-1)$ and we have with $\hat A_{0,j}:=A_0\sigma^{j\hat\alpha}$, $\hat A_{1,j}:=A_1\sigma^{-j}$

$$\forall x\in I_j\quad\forall k\geq 2:\qquad \left|D^kg(x)\right|\leq\hat A_{0,j}\hat A_{1,j}^k(k!)^\delta. \tag{2.10}$$

We now apply Theorem 2.3 to $Q_n^{I_j}g$. Note that in the proof of Theorem 2.3 only derivatives $g^{(k)}$ with $k\geq 2$ were used and that the constants C,r in (2.3) depend only on δ and $\rho=\hat A_{1,j}\ell_j/2=A_1(\sigma^{-1}-1)/2$. As ρ is independent of j we obtain with the same $C,r>0$ for $j=1,\ldots,m-1$

$$\left|\mathcal{I}^{I_j}g-Q_n^{I_j}g\right|\leq\hat A_{0,j}\ell_jC\exp(-rn^{1/\delta})=A_0\sigma^{j(\hat\alpha+1)}(\sigma^{-1}-1)C\exp(-rn^{1/\delta}) \tag{2.11}$$

$$\sum_{j=1}^{m-1}\left|\mathcal{I}^{I_j}g-Q_n^{I_j}g\right|\leq A_0\frac{\sigma^{-1}-1}{\sigma^{-\hat\alpha-1}-1}C\exp(-rn^{1/\delta}) \tag{2.12}$$

where we could add the geometric series for $j=1,\ldots,\infty$ as $\hat\alpha>-1\implies\sigma^{\hat\alpha+1}\in(0,1)$.

For $j=m$ we let $\alpha_0:=\min(\alpha,0)>-1$ and $f(x):=A_0x^{\alpha_0}$, then $|g(x)|\leq f(x)$ and $\left|Q_n^{I_m}g\right|\leq Q_n^{I_m}f$. Remark 4 in [5] shows that $Q_n^{I_m}f$ converges as $n\to\infty$ and $Q_n^{I_m}f\leq c_{\alpha_0}\mathcal{I}^{I_m}f$. Hence

$$\left|\mathcal{I}^{I_m}g-Q_n^{I_m}g\right|\leq\left|\mathcal{I}^{I_m}g\right|+\left|Q_n^{I_m}g\right|\leq(1+c_{\alpha_0})\mathcal{I}^{I_m}f=c\int_0^{\sigma^{m-1}}x^{\alpha_0}\mathrm{d}x=c'\sigma^{(m-1)(\alpha_0+1)}. \tag{2.13}$$

Combining this with (2.12) gives

$$|\mathcal{I}g - Q_{n,m,\sigma}g| \le \sum_{j=1}^{m} \left|\mathcal{I}^{I_j}g - Q_n^{I_j}g\right| \le C' \exp(-rn^{1/\delta}) + C''\sigma^{(m-1)(\alpha_0+1)}.$$

Choosing $m = \lceil bn^{1/\delta} \rceil$ then gives (2.9). □

Remark 2.6. Note that we have to know the value of the Gevrey parameter δ to obtain the rate $C\exp(-rN^{1/(1+\delta)})$. If we do not know the value of δ we can choose $m = cn$ (as in the case $\delta = 1$) and obtain $N = O(n^2)$ and

$$|\mathcal{I}g - Q_{n,m}g| \le c' \exp(-rn^{1/\delta}) + c'' \exp(-r'm) \le C\ \exp(-\tilde{r}N^{1/(2\delta)})$$

which is worse than $C\exp(-rN^{1/(1+\delta)})$ for $\delta > 1$ (but still gives exponential convergence).

We now consider the convergence rate of the variable order composite Gauss rule.

Theorem 2.7. *Assume that $g \in G^{\delta,\alpha}([0,1])$ with $\delta \ge 1$, $\alpha > -1$. Let $\sigma \in (0,1)$, $b > 0$. Then the variable order composite rule $Q_{n,m,\sigma,\delta}$ with $m = \lceil bn^{1/\delta} \rceil$ has a total number of evaluation points $N = O(n^{1+\delta^{-1}})$ and there exist $C, r, r' > 0$ such that for all $n \in \mathbb{N}$*

$$|\mathcal{I}g - Q_{n,m,\sigma,\delta}g| \le C\exp(-r'n^{1/\delta}) \le C\exp(-rN^{1/(1+\delta)}). \tag{2.14}$$

Proof. We proceed as in the proof of Theorem 2.5 and obtain for $j = 1, \dots, m-1$ using $n_j \ge nm^{-\delta}(m+1-j)^\delta$

$$\left|\mathcal{I}^{I_j}g - Q_{n_j}^{I_j}g\right| \le A_0\sigma^{j(\hat{\alpha}+1)}(\sigma^{-1}-1)C\exp(-rn_j^{1/\delta}) \le c\sigma^{j(\hat{\alpha}+1)}\exp\left(-rn^{1/\delta}m^{-1}(m+1-j)\right) =: E_j \tag{2.15}$$
$$E_1 = c\sigma^{\hat{\alpha}+1}\exp(-rn^{1/\delta}), \qquad E_{m-1} = c\sigma^{(m-1)(\hat{\alpha}+1)}\exp(-rn^{1/\delta}2m^{-1}) \le c\sigma^{(m-1)(\hat{\alpha}+1)}.$$

As E_j is of the form $E_j = aq^j$ we have

$$\sum_{j=1}^{m-1} E_j \le (m-1)\max_{j=1,\dots,m-1} E_j \le (m-1)\max\{E_1, E_{m-1}\} \le C(m-1)\max\left\{\exp(-rn^{1/\delta}), \sigma^{m(\hat{\alpha}+1)}\right\}. \tag{2.16}$$

For $j = m$ we use (2.13). Combining this with (2.11), (2.16) yields

$$|\mathcal{I}g - Q_{n,m,\sigma,\delta}g| \le \sum_{j=1}^{m}\left|\mathcal{I}^{I_j}g - Q_{n_j}^{I_j}g\right| \le C(m-1)\max\{\exp(-rn^{1/\delta}), \sigma^{m(\hat{\alpha}+1)}\} + C\sigma^{m(\alpha_0+1)}$$

and using $bn^{1/\delta} \le m \le bn^{1/\delta} + 1$ gives $|\mathcal{I}g - Q_{n,m,\sigma,\delta}g| \le C_{r'}\exp(-r'n^{1/\delta})$ with $r' < r$. □

2.4. Tensor product quadrature on $[0,1]^d$

Proposition 2.8. *Let $d \in \mathbb{N}$, $\delta \ge 1$, $\alpha > -1$ and assume $g \in G^{\delta,\alpha}_{\{1\}}([0,1]^d)$. Let $\sigma \in (0,1)$, $b > 0$, $m = \lceil bn^{1/\delta} \rceil$ and $Q_{n,m}$ as in Definition 2.4. Then there exist $C, r, r' > 0$ such that for all $n \in \mathbb{N}$*

$$\left|\int_{\zeta\in[0,1]^d} g(\zeta)\,\mathrm{d}\zeta - Q_{n,m} \otimes \underbrace{Q_n \otimes \cdots \otimes Q_n}_{d-1\ \ times} g\right| \le C\exp(-rn^{1/\delta}) \le C\exp(-r'N^{1/(\delta d+1)}). \tag{2.17}$$

Here $N = (\sum_{j=1}^m n_j)n^{d-1} = O(n^{d+\delta^{-1}})$ is the total number of quadrature points.

Proof. We use induction over d. For $d = 1$ the result is given by Theorem 2.5. For $d \geq 2$ we let $\zeta' := (\zeta_1, \dots, \zeta_{d-1})$ and define $\tilde{g}(\zeta') := Q_n g(\zeta', \cdot)$, $h(\zeta_d) := \int_{\zeta' \in [0,1]^{d-1}} g(\zeta) \mathrm{d}\zeta'$. Then

$$\int_{\zeta \in [0,1]^d} g(\zeta)\mathrm{d}\zeta - Q_{n,m} \otimes \underbrace{Q_n \otimes \cdots \otimes Q_n}_{d-1 \text{ times}} g = \left(\int_{\zeta' \in [0,1]^{d-1}} \tilde{g}(\zeta')\mathrm{d}\zeta' - Q_{n,m} \otimes \underbrace{Q_n \otimes \cdots \otimes Q_n}_{d-2 \text{ times}} \tilde{g} \right) + \left(\int_{\zeta_d=0}^{1} h(\zeta_d)\mathrm{d}\zeta_d - Q_n h \right) =: T_1 + T_2. \tag{2.18}$$

For T_1 we note that $\left|D^\beta \tilde{g}(\zeta')\right| \leq \max_{\zeta_d \in [0,1]} \left|D^{(\beta,0)} g(\zeta)\right|$ as Q_n has positive weights with sum 1. Hence $g \in G^{\delta,\alpha}_{\{1\}}([0,1]^d)$ implies $\tilde{g} \in G^{\delta,\alpha}_{\{1\}}([0,1]^{d-1})$ and the induction assumption gives $|T_1| \leq C \exp(-rn^{1/\delta})$.

For T_2 we note that

$$\left|D^k h(\zeta_d)\right| \leq \int_{\zeta' \in [0,1]^{d-1}} \left|D^{(0,\dots,0,k)} g(\zeta)\right| \mathrm{d}\zeta' \leq \int_{\zeta' \in [0,1]^{d-1}} A_0 A_1^k (k!)^\delta \left|\zeta_1\right|^{\min\{0,\alpha\}} \mathrm{d}\zeta' \leq \tilde{A}_0 A_1^k (k!)^\delta$$

so that $h \in G^\delta([0,1])$. Hence Theorem 2.3 gives $|T_2| \leq C \exp(-rn^{1/\delta})$. □

Remark 2.9. In the case of $g \in G^\delta([0,1]^d)$ with $d \in \mathbb{N}$, $\delta \geq 1$ we can use standard tensor product Gaussian quadrature and obtain in the same way the result

$$\left| \int_{\zeta \in [0,1]^d} g(\zeta)\, \mathrm{d}\zeta - \underbrace{Q_n \otimes \cdots \otimes Q_n}_{d \text{ times}} g \right| \leq C \exp(-rn^{1/\delta}) \leq C \exp(-r' N^{1/(\delta d)})$$

where $N = n^d$ is the total number of quadrature points.

3. Quadrature of singular functions on simplices

3.1. Introduction

We want to compute the integral

$$I = \int_{x \in S^{(1)}} \int_{y \in S^{(2)}} g(x,y)\, \mathrm{d}y\, \mathrm{d}x \tag{3.1}$$

where we make the following assumptions:

Assumption 3.1. *$S^{(1)}, S^{(2)} \subset \mathbb{R}^d$ are d-dimensional closed simplices with positive volume. Moreover, $S^{(1)} \cap S^{(2)}$ is either empty, or a k-dimensional simplex side with $k \in \{0, \dots, d\}$,* i.e., *the convex hull of $k+1$ common vertices of $S^{(1)}, S^{(2)}$.*

Assumption 3.1 is satisfied if $S^{(j)}$ are simplices in a regular finite element mesh.

Assumption 3.2. *The function $g(x,y)$ can be written as $g(x,y) = F(x,y,y-x)$ with $F \in G^{\delta,\alpha}_{\{2d+1,\dots,3d\}}(S^{(1)} \times S^{(2)} \times (S^{(2)} - S^{(1)}))$ with $\delta \geq 1$, $\alpha \in \mathbb{R}$: There exist A_0, A_1 so that for all $\beta = (\beta_x, \beta_y, \beta_z) \in \mathbb{N}_0^{3d}$, $x \in S^{(1)}$, $y \in S^{(2)}$, $z \in S^{(2)} - S^{(1)}$*

$$\left|D^\beta F(x,y,z)\right| \leq A_0 A_1^{|\beta|} (\beta!)^\delta \left\|z\right\|^{\min(\alpha - |\beta_z|, 0)}.$$

If $S^{(1)} \cap S^{(2)}$ is nonempty we assume $\alpha > k - 2d$, this implies $g \in L^1(S^{(1)} \times S^{(2)})$.

We want to rewrite this integral in the form of nested one-dimensional integrals. Then we will approximate the one-dimensional integrals either by Gauss quadrature or by composite Gauss quadrature. To this end, we define the standard simplex in $\mathbb{R}^d$ by

$$S_d := \{(x_1, \ldots, x_d) \mid x_j \geq 0,\, x_1 + \ldots + x_d \leq 1\}. \tag{3.2}$$

Let us denote the vertices of $S^{(j)}$ by $v^{(j,0)}, \ldots, v^{(j,d)}$, let $w^{(j,k)} := v^{(j,k)} - v^{(j,0)}$ for $j = 1, 2$ and $k = 1, \ldots, d$. We define $A^{(j)} := (w^{(j,1)}, \ldots, w^{(j,d)}) \in \mathbb{R}^{d\times d}$ and use the change of variables from $x \in S^{(1)}, y \in S^{(2)}$ to $u, v \in S_d$ given by

$$x = v^{(1,0)} + A^{(1)}u, \qquad y = v^{(2,0)} + A^{(2)}v \tag{3.3}$$

yielding

$$G(u, v) := g\left(v^{(1,0)} + A^{(1)}u, v^{(2,0)} + A^{(2)}v\right) \left|\det A^{(2)} \det A^{(1)}\right| \tag{3.4}$$

$$I = \int_{x\in S^{(1)}} \int_{y\in S^{(2)}} g(x, y)\mathrm{d}y\,\mathrm{d}x = \int_{u\in S_d} \int_{v\in S_d} G(u, v)\,\mathrm{d}v\,\mathrm{d}u. \tag{3.5}$$

If the intersection $S^{(1)} \cap S^{(2)}$ is empty the simplices have a distance $D > 0$. Then the new integrand $G(u, v)$ is Gevrey regular on $S_d \times S_d$. Using the coordinates $\xi_j = (1 - u_1 - \ldots - u_{j-1})^{-1}u_j$ for $j = 1, \ldots, d$ we have $u = \Psi(\xi) := (\xi_1, (1 - \xi_1)\xi_2, \ldots, (1 - \xi_1)\ldots(1 - \xi_{d-1})\xi_d)$ and $J_\Psi(\xi) = \prod_{j=1}^{d-1}(1 - \xi_j)^{d-j}$ so that

$$I = \int_{\xi\in[0,1]^d} \int_{\eta\in[0,1]^d} \tilde{G}(\xi, \eta)\,\mathrm{d}\eta\,\mathrm{d}\xi, \qquad \tilde{G}(\xi, \eta) := G(\Psi(\xi), \Psi(\eta))J_\Psi(\xi)J_\Psi(\eta).$$

We can now use Gaussian quadrature and obtain exponential convergence:

Proposition 3.3. *The function $\tilde{G}$ satisfies $\tilde{G} \in G^\delta([0, 1]^{2d})$. As a consequence we have for the quadrature error with $C, r > 0$*

$$\left|I - Q_n \otimes \cdots \otimes Q_n(\tilde{G})\right| \leq C \exp(-rn^{1/\delta}) = C \exp(-rN^{1/(2\delta d)}).$$

Proof. The result follows from Corollary 4.9 in the next section and Remark 2.9. □

Note that for a shape regular finite element mesh we have $D \geq c \max\{\operatorname{diam} S^{(1)}, \operatorname{diam} S^{(2)}\}$ with fixed c, even for non-quasi uniform meshes. Hence we obtain a uniform $r > 0$ for the convergence.

If the intersection $S^{(1)} \cap S^{(2)}$ is nonempty and k-dimensional with $k \in \{0, \ldots, d\}$ we can number the vertices of the simplices so that $v^{(1,j)} = v^{(2,j)}$ for $j = 0, \ldots, k$, $v^{(1,j)} \neq v^{(2,j)}$ for $j = k + 1, \ldots, d$. We now want to describe the regularity of the function G given by (3.4).

Remember that $g(x, y) = F(x, y, y - x)$ with $F \in G^{\delta,\alpha}_{\{2d+1,\ldots,3d\}}(S^{(1)}, S^{(2)}, S^{(2)} - S^{(1)})$. Hence we have in (3.5)

$$G(u, v) = c \cdot F\left(v^{(1,0)} + A^{(1)}u, v^{(1,0)} + A^{(2)}v, A^{(2)}v - A^{(1)}u\right) \tag{3.6}$$

as $v^{(1,0)} = v^{(2,0)}$. Moreover, the first k columns of $A^{(1)}, A^{(2)}$ coincide so that $A^{(j)} = (B, B^{(j)})$ with $B \in \mathbb{R}^{d\times k}$, $B^{(j)} \in \mathbb{R}^{d\times(d-k)}$. Let $\hat{u} := (u_1, \ldots, u_k)^\top$, $\check{u} := (u_{k+1}, \ldots, u_d)^\top$ and similarly for v, then (3.3) gives

$$x = v^{(1,0)} + B\hat{u} + B^{(1)}\check{u}, \qquad y = v^{(1,0)} + B\hat{v} + B^{(2)}\check{v}, \tag{3.7}$$

$$y - x = A^{(2)}v - A^{(1)}u = B(\hat{v} - \hat{u}) + B^{(2)}\check{v} - B^{(1)}\check{u}. \tag{3.8}$$

By a *closed cone* we denote a closed subset X of $\mathbb{R}^d$ with the property $x \in X \implies \alpha x \in X$ for all $\alpha \geq 0$. For $u^{(1)}, \ldots, u^{(m)} \in \mathbb{R}^d$ we define $\operatorname{cone}\{u^{(1)}, \ldots, u^{(m)}\} := \{\, c_1u^{(1)} + \ldots + c_mu^{(m)} \mid c_j \geq 0 \,\}$.

Proposition 3.4. *Let X, Y be closed cones in $\mathbb{R}^d$ with $X \cap Y = \{0\}$. Then there exists $c_{X,Y} > 0$ such that*

$$\forall x \in X,\, \forall y \in Y: \qquad \|x-y\|^2 \geq c_{X,Y}\left(\|x\|^2 + \|y\|^2\right).$$

Proof. Let $X_1 = \{x \in X \mid \|x\| = 1\}$ and Y_1 defined analogously. Since $X_1 \times Y_1$ is compact and $X_1 \cap Y_1 = \{\}$ the inner product (x, y) has on $X_1 \times Y_1$ a maximum $1-\varepsilon$ with $\varepsilon > 0$. Now let $x \in X$ and $y \in Y$. Then $(x, y) \leq (1-\varepsilon)\|x\|\,\|y\|$ and

$$\|x-y\|^2 = \|x\|^2 - 2(x,y) + \|y\|^2 \geq \|x\|^2 - 2(1-\varepsilon)\|x\|\,\|y\| + \|y\|^2 \geq \varepsilon\left(\|x\|^2 + \|y\|^2\right)$$

using $2\|x\|\,\|y\| \leq \|x\|^2 + \|y\|^2$. □

We define the closed cones

$$V := \operatorname{span}\{w^{(1,1)}, \ldots, w^{(1,k)}\}, \qquad X^{(1)} := \operatorname{cone}\{w^{(1,k+1)}, \ldots, w^{(1,d)}\}, \qquad X^{(2)} := \operatorname{cone}\{w^{(2,k+1)}, \ldots, w^{(2,d)}\}$$

and have that $S^{(j)} \subset v^{(1,0)} + V + X^{(j)}$ for $j = 1, 2$. Let $x \in S^{(1)}$, $y \in S^{(2)}$, then (3.7) gives the decompositions

$$x = v^{(1,0)} + x^{(0)} + x^{(1)}, \qquad y = v^{(1,0)} + y^{(0)} + y^{(2)}, \qquad x^{(0)} := B\hat{u}, \quad x^{(1)} := B^{(1)}\check{u}, \quad y^{(0)} := B\hat{v}, \quad y^{(2)} := B^{(2)}\check{v}$$

with $x^{(0)}, y^{(0)} \in V$, $x^{(1)} \in X^{(1)}$, $y^{(2)} \in X^{(2)}$. By the assumptions on the simplices $S^{(1)}, S^{(2)}$ we have $X^{(1)} \cap \left(V + X^{(2)}\right) = \{0\}$ and $V \cap X^{(2)} = \{0\}$, hence Proposition 3.4 yields

$$\begin{aligned}\|y-x\|^2 = \left\|\left(y^{(2)} + y^{(0)} - x^{(0)}\right) - x^{(1)}\right\|^2 &\geq c\left(\left\|y^{(2)} - \left(x^{(0)} - y^{(0)}\right)\right\|^2 + \left\|x^{(1)}\right\|^2\right)\\ &\geq c'\left(\left\|y^{(2)}\right\|^2 + \left\|x^{(0)} - y^{(0)}\right\|^2 + \left\|x^{(1)}\right\|^2\right)\end{aligned}$$

$$\|y-x\|^2 \geq c'\left(\|B(\hat{v}-\hat{u})\|^2 + \left\|B^{(1)}\check{u}\right\|^2 + \left\|B^{(2)}\check{v}\right\|^2\right) \geq c''\left(\|\hat{v}-\hat{u}\|^2 + \|\check{u}\|^2 + \|\check{v}\|^2\right) \tag{3.9}$$

since the columns of $B, B^{(1)}, B^{(2)}$ are linearly independent. We assumed that $g(x, y) = F(x, y, y-x)$ with $F \in G^{\delta,\alpha}_{\{2d+1,\ldots,3d\}}(S^{(1)} \times S^{(2)} \times (S^{(2)} - S^{(1)}))$, so (3.6) gives $G(u, v) = H(u, v, \hat{v}-\hat{u}, \check{u}, \check{v})$ with

$$H(u, v, \xi, \eta, \zeta) := c \cdot F\left(v^{(1,0)} + A^{(1)}u, v^{(1,0)} + A^{(2)}v, B\xi + B^{(2)}\zeta - B^{(1)}\eta\right). \tag{3.10}$$

Let $w := B\xi + B^{(2)}\zeta - B^{(1)}\eta$, then (3.9) gives $\|w\| \geq c\,\|(\xi, \eta, \zeta)\|$. Hence we obtain with $\beta = (\beta_u, \beta_v, \beta_\xi, \beta_\eta, \beta_\zeta)$

$$\left|D^\beta H(u, v, \xi, \eta, \zeta)\right| \leq \tilde{A}_0\tilde{A}_1^\beta(\beta!)^\delta\,\|w\|^{\min(\alpha-|\beta_\xi|-|\beta_\eta|-|\beta_\zeta|,0)} \leq \check{A}_0\check{A}_1^\beta(\beta!)^\delta\,\|(\xi, \eta, \zeta)\|^{\min(\alpha-|\beta_\xi|-|\beta_\eta|-|\beta_\zeta|,0)}$$

so that

$$G(u, v) = H(u, v, \hat{v}-\hat{u}, \check{u}, \check{v}), \qquad H \in G^{\delta,\alpha}_{\{2d+1,\ldots,4d-k\}}\left(S_d \times S_d \times (S_k - S_k) \times S_{d-k} \times S_{d-k}\right). \tag{3.11}$$

Our goal is to rewrite integral I as

$$I = \int_{u \in S_d}\int_{v \in S_d} G(u, v)\,\mathrm{d}v\,\mathrm{d}u = \sum_{i=1}^{K}\int_{[0,1]^{2d}} \tilde{G}_j(\zeta)\mathrm{d}\zeta$$

so that the new integrands satisfy $\tilde{G}_j \in G^{\delta,\tilde{\alpha}}_{\{1\}}([0,1]^{2d})$, *i.e.*, $\tilde{G}_j(\zeta)$ is only singular with respect to ζ_1 at $\zeta_1 = 0$. This will allow us to use composite Gauss quadrature for ζ_1, and standard Gauss quadrature for the variables $\zeta_2, \ldots, \zeta_{2d}$.

We will first derive some useful tools, and then state the transformations and their properties.

3.2. Tools

The standard simplex (3.2) can be parameterized by $(x_1, \ldots, x_d)$ as follows:

$$x \in S_d \iff x_j \in \left[0, 1 - \sum_{i=1}^{j-1} x_i\right] \text{ for } j = 1, \ldots, d. \tag{3.12}$$

$$\int_{x \in S_d} f(x)\mathrm{d}x = \int_{x_1=0}^{1} \int_{x_2=0}^{1-x_1} \cdots \int_{x_d=0}^{1-x_1-\ldots-x_{d-1}} f(x)\mathrm{d}x_d \ldots \mathrm{d}x_2 \mathrm{d}x_1. \tag{3.13}$$

Here we allow in parameterizations that the bounds for a variable depend on previous variables (so that we can write integrals as nested one-dimensional integrals). In the sequel we will leave integrals in the form $\int_{x \in S_d} f(x)\mathrm{d}x$, it is then implicitly understood that they can be expressed as an iterated integral using (3.13). For a vector $v = (v_1, \ldots, v_k)$ we will use the notations $v' := (v_1, \ldots, v_{k-1})$, $\sum_j v_j = v_1 + \ldots + v_k$, $\sigma_v := 1 - \sum_j v_j$.

We now define a pyramid $P(B) \in \mathbb{R}^d$ with base B: Consider a $(d-1)$ dimensional hyperplane not containing 0 and let B be a subset. Then define

$$P(B) := \{sx \mid s \in [0,1],\ x \in B\}. \tag{3.14}$$

With a parameterization $B = \{(x', q(x')) \mid x' \in B'\}$ with $B' \subset \mathbb{R}^{d-1}$ and an affine function q we can write

$$\int_{x \in P(B)} f(x)\mathrm{d}x = \int_{s=0}^{1} \int_{x' \in B'} f\left(s\left(x', q(x')\right)\right) s^{d-1} \mathrm{d}x' \, \mathrm{d}s.$$

E.g., we have $S_d = P(B_d)$ with the base

$$B_d := \{(x_1, \ldots, x_d) \mid x_j \geq 0,\ \sum_j x_j = 1\} = \{(x_1, \ldots, x_{d-1}, 1 - x_1 - \ldots - x_{d-1}) \mid (x_1, \ldots, x_{d-1}) \in S_{d-1}\}. \tag{3.15}$$

This gives another parameterization for S_d:

$$\int_{x \in S_d} f(x)\mathrm{d}x = \int_{s=0}^{1} \int_{x' \in S_{d-1}} f\left(s\left(x', \sigma_{x'}\right)\right) s^{d-1} \mathrm{d}x' \, \mathrm{d}s. \tag{3.16}$$

We will also encounter integrals over a domain $P(B_m \times S_n) \subset \mathbb{R}^{m+n}$: In this case we obtain with $x \in \mathbb{R}^m$, $y \in \mathbb{R}^n$ that

$$\int_{(x,y) \in P(B_m \times S_n)} f(x,y)\, \mathrm{d}y\, \mathrm{d}x = \int_{s=0}^{1} \int_{x' \in S_{m-1}} \int_{y \in S_n} f\left(s\left(x', \sigma_{x'}, y\right)\right) s^{m+n-1} \mathrm{d}y\, \mathrm{d}x'\, \mathrm{d}s. \tag{3.17}$$

We now consider a Cartesian product of m pyramids and split it into m pyramids:

Proposition 3.5. *Let $D = P(B_{(1)}) \times \ldots \times P(B_{(m)}) \in \mathbb{R}^{d_1 + \ldots + d_m}$ where $B_{(j)}$ is a $(d_j - 1)$-dimensional base in $\mathbb{R}^{d_j}$. Then*

$$D = \tilde{D}_1 \cup \ldots \cup \tilde{D}_j, \qquad \mathrm{meas}(\tilde{D}_i \cap \tilde{D}_j) = 0, \qquad i, j \in \{1, \ldots, m\}, \quad i \neq j \tag{3.18}$$

where $\tilde{D}_j = P(\tilde{B}_{(j)})$ with

$$\tilde{B}_{(j)} = P(B_{(1)}) \times \ldots \times P(B_{(j-1)}) \times B_{(j)} \times P(B_{(j+1)}) \times \ldots \times P(B_{(m)}). \tag{3.19}$$

Proof. We have $P(B_j) := \{t^{(j)}x^{(j)} \mid t^{(j)} \in [0,1],\ x^{(j)} \in B_j\}$ and $D = \tilde{D}_1 \cup \ldots \cup \tilde{D}_m$ with

$$\begin{aligned}\tilde{D}_1 &= \left\{(t^{(1)}x^{(1)}, \ldots, t^{(m)}x^{(m)}) \mid t^{(j)} \in [0,1],\, x^{(j)} \in B_{(j)},\, \max_j t^{(j)} = t^{(1)}\right\} \\ &= \left\{s\left(x^{(1)}, t^{(2)}x^{(2)}, \ldots, t^{(m)}x^{(m)}\right) \mid s \in [0,1],\, t^{(j)} \in [0,1],\, x^{(j)} \in B_{(j)}\right\} = P\left(B_{(1)} \times P(B_{(2)}) \times \cdots \times P(B_{(m)})\right)\end{aligned} \tag{3.20}$$

and correspondingly for $\tilde{D}_2, \ldots, \tilde{D}_m$. □

We apply for $(x,y) \in S_d \times S_d$ the transformation $(x,y) = (x, x+z)$ with $z = y - x \in S_d - S_d$ and $x \in S_d$ such that $y = x + z \in S_d$: let $A_d := S_d - S_d$ and $E_d(z) := S_d \cap (S_d - z)$, then

$$S_d \times S_d = \{(x, x+z) \mid z \in A_d,\ x \in E_d(z)\}.$$

The idea of introducing the coordinates $z = y - x$ goes back to [9] in dimension $d = 1$ and was extended to the case of boundary integral operators on surfaces in $\mathbb{R}^3$ in [18]; see also Chapter 5 of [19] for an account of this.

Note that $E_d(z)$ is always similar to S_d: we have $x \in E_d(z)$ iff

$$x_k \geq \max\{0, -z_k\} \quad \text{and} \quad \sum_j x_j \leq 1 - \max\left\{0, \sum_j z_j\right\}. \tag{3.21}$$

Note that this yields a parameterization with the variables $x_1, \ldots, x_d$ where the lower bound for each variable is given by the left inequality, and the upper bound (in terms of the previous variables) by the right inequality. Recall the definitions of x_N and $x^{(N)}$ for $N \subset \{1, \ldots, d\}$ and $x \in \mathbb{R}^d$ from section 1.1.

We now show that we can split A_d into pyramids $A^{\pm}_{N,M\setminus N} = P(B^{\pm}_{N,M\setminus N})$. This is illustrated in Figure 1 for $d = 2$ and $d = 3$ dimensions. In the algorithm we will use the bases $B^{+}_{N,M\setminus N}$ for all subsets $N \subset M$. Note that we can visualize these bases flattened into $\mathbb{R}^{d-1}$ as shown in Figure 2 for $d = 3, 4$. For $\#N = j$ equation (3.24) shows that $B^{+}_{N,M\setminus N}$ is a Cartesian product of a j-dimensional simplex and a $d - j - 1$-dimensional simplex. Consider the case $d = 4$: For $j = 0$ we have $\binom{4}{0} = 1$ base which is (0-simplex) × (3-simplex) (tetrahedron), for $j = 1$ we have $\binom{4}{1} = 4$ bases which are (1-simplex) × (2-simplex) (prisms), for $j = 2$ we have $\binom{4}{2} = 6$ bases which are (2-simplex) × (1-simplex) (prisms), for $j = 3$ we have $\binom{4}{3} = 4$ bases which are (3-simplex) × (0-simplex) (tetrahedra).

Lemma 3.6. *We have with $M = \{1, \ldots, d\}$*

$$A_d = \bigcup_{N \subset M} A_{N,M\setminus N}, \qquad A_{N^-,N^+} := \{z \in A_d \mid z_{N^-} \leq 0,\ z_{N^+} \geq 0\} = \left\{z \mid z_{N^-} \in -S_{\#N^-},\ z_{N^+} \in S_{\#N^+}\right\}. \tag{3.22}$$

If $N = \{\}$

$$z \in A_{\{\},\{1,\ldots,d\}} = S_d \quad \Longrightarrow \quad E_d(z) = (1 - z_1 - \ldots - z_d)S_d.$$

If $N = M$

$$z \in A_{\{1,\ldots,d\},\{\}} = -S_d \quad \Longrightarrow \quad E_d(z) = -z + (1 + z_1 + \ldots + z_d)S_d.$$

If $N \neq \{\}$ and $N \neq M$ we have that $A_{N,M\setminus N}$ is a Cartesian product of two pyramids with bases $x_N \in -B_{\#N}$ and $x_{M\setminus N} \in B_{\#(M\setminus N)}$. Hence we can split it into two pyramids using $A_{N,M\setminus N} = A^{+}_{N,M\setminus N} \cup A^{-}_{N,M\setminus N}$ where

$$A^{+}_{N^-,N^+} := \{z \in A_{N^-,N^+} \mid \textstyle\sum_j z_j \geq 0\} = \left\{sz \mid z_{N^-} \in -tB_{\#N^-},\ z_{N^+} \in B_{\#N^+};\ s,t \in [0,1]\right\} = P(B^{+}_{N^-,N^+}) \tag{3.23}$$

$$B^{+}_{N^-,N^+} := \left\{x \mid x_{N^-} \in -S_{\#N^-},\ x_{N^+} \in B_{\#N^+}\right\} \tag{3.24}$$

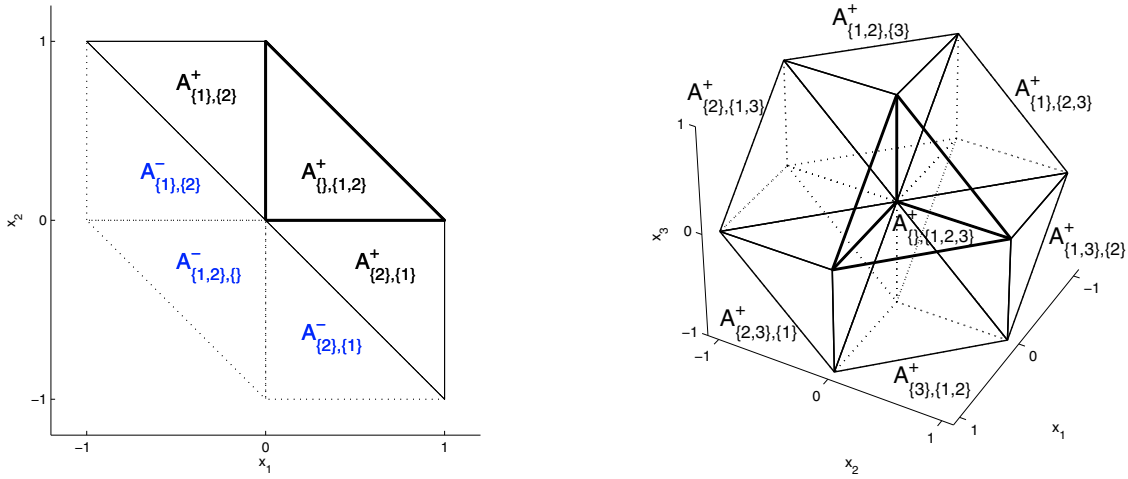

FIGURE 1. The domain $A_d = \bigcup_{N \subset M} \bigcup_{\sigma \in \{+,-\}} A^{\sigma}_{N,M\setminus N}$ for $d = 2$ (left) and $d = 3$ (right, only labeled for $\sigma = +$).

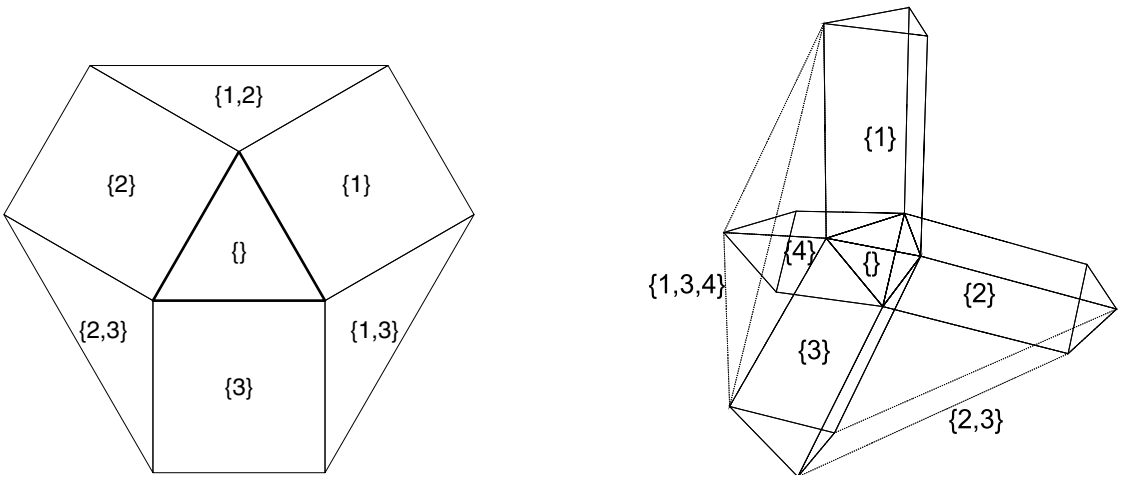

FIGURE 2. The bases $B^{+}_{N,M\setminus N}$ flattened into $\mathbb{R}^{d-1}$ for $d = 3$ (left) and $d = 4$ (right) and labeled with N. For $d = 4$ only 1 of 6 bases with $\#N = 2$ and 1 of 4 bases with $\#N = 3$ are shown with dotted lines.

$$A^{-}_{N^-,N^+} := \{z \in A_{N^-,N^+} \mid \textstyle\sum_j z_j \le 0\} = \big\{sz \mid z_{N^-} \in -B_{\#N^-},\, z_{N^+} \in tB_{\#N^+};\, s,t \in [0,1]\big\} = P(B^{-}_{N^-,N^+}) \tag{3.25}$$

$$B^{-}_{N^-,N^+} := \big\{x \mid x_{N^-} \in -B_{\#N^-},\, x_{N^+} \in S_{\#N^+}\big\} \tag{3.26}$$

$$z \in A^{+}_{N^-,N^+} \quad \Longrightarrow \quad E_d(z) = -z^{(N^-)} + \left(1 - \sum_j (z_{N^+})_j\right) S_d \tag{3.27}$$

$$z \in A^{-}_{N^-,N^+} \quad \Longrightarrow \quad E_d(z) = -z^{(N^-)} + \left(1 + \sum_j (z_{N^-})_j\right) S_d. \tag{3.28}$$

Proof. In (3.22) we split A_d into the parts belonging to the 2^d octants in $\mathbb{R}^d$. It remains to show the rightmost equality in (3.22): If $z \in S_d - S_d$ with $z_{N^-} \le 0$ and $z_{N^+} \ge 0$ we have to show that $\sum_j (z_{N^-})_j \ge -1$ and $\sum_j (z_{N^+})_j \le 1$. But if $z = y - x$ with $x, y \in S_d$ we have with $z^\pm := z_{N^\pm}$ and correspondingly for x, y

$$\sum_j z_j^- = \sum_j y_j^- - \sum_j x_j^- \ge \sum_j y_j^- - \left(1 - \sum_j x_j^+\right) \ge -1$$

$$\sum_j z_j^+ = \sum_j y_j^+ - \sum_j x_j^+ \le \left(1 - \sum_j y_j^-\right) - \sum_j x_j^+ \le 1.$$

It is also clear that one can obtain *all* points $z^- \in -S_{\#N^-}$ and $z^+ \in S_{\#N^+}$ in this way by choosing $x, y \in S_d$ as follows:

$$y_{N^-} = 0, \quad y_{N^+} = z^+, \quad x_{N^-} = -z^-, \quad x_{N^+} = 0.$$

For the right equality in (3.23) we use that $\sum_j z_j \ge 0 \iff \sum_j (-z_j^-) \le \sum z_j^+$, and then we apply (3.20). The statements about $E_d(z)$ follow in each case directly from (3.21): for $z \in A^+_{N^-,N^+}$ we have $z_{N^-} \le 0$, $z_{N^+} \ge 0$, therefore $x_k \ge \max\{0, -z_k\}$ is equivalent to $x \ge -z^{(N^-)}$. We also have $z_1 + \ldots + z_d \ge 0$, so $\sum_j x_j \le 1 - \max\{0, \sum_j z_j\}$ is equivalent to $\sum_j x_j \le 1 - z_1 - \ldots - z_d = 1 - \sum_j (z_{N^-})_j - \sum_j (z_{N^+})_j$. Therefore $v := x + z^{(N^-)}$ satisfies $v \ge 0$ and $\sum_j v_j \le 1 - \sum_j (z_{N^+})_j$. The other cases follow in the same way. □

Let $A^+_{\{\},M} := A_{\{\},M} = S_d$, $A^-_{\{\},M} := \{\}$, $A^-_{M,\{\}} := A_{M,\{\}} = -S_d$, $A^+_{M,\{\}} := \{\}$ and define

$$E^\pm_{N^-,N^+}(z) := -z^{(N^-)} + \left(1 \mp \sum_j (z_{N^\pm})_j\right) S_d. \tag{3.29}$$

Then we can state the result as follows:

$$\int_{x\in S_d} \int_{y \in S_d} f(x,y)\,\mathrm{d}y\,\mathrm{d}x = \sum_{N\subset M} \sum_{\sigma\in\{-,+\}} \int_{z\in A^\sigma_{N,M\setminus N}} \int_{x\in E^\sigma_{N,M\setminus N}(z)} f(x, x+z)\,\mathrm{d}x\,\mathrm{d}z. \tag{3.30}$$

This is a sum over $2^d \cdot 2$ terms, but two of the $A^\sigma_{N,M\setminus N}$ are empty so that only $2^{d+1} - 2$ terms remain. Recall that all the domains $A^\sigma_{N,M\setminus N}$ are pyramids in $\mathbb{R}^d$ with apex in the origin. For $z \in A^\sigma_{N,M\setminus N}$ we use the parameterization with the variables (s, t, z_{N^-}, z_{N^+}) from (3.23), (3.25) where (3.15) is used for z_{N^-}, z_{N^+}. For $x \in E^\sigma_{N,M\setminus N}(z)$ we can simply use the variables $x_1, \ldots, x_d$.

3.3. Transformations

For $x \in \mathbb{R}^d$ we write $x = (\hat{x}, \check{x})$ with $\hat{x} = (x_1, \ldots, x_k)$ and $\check{x} = (x_{k+1}, \ldots, x_d)$.

From (3.5) we obtain the integral

$$I = \int_{x\in S_d} \int_{y\in S_d} G(x,y)\mathrm{d}y\,\mathrm{d}x, \tag{3.31}$$

where G satisfies (3.11). Hence the function G is Gevrey smooth unless $(\hat{y} - \hat{x}, \check{x}, \check{y}) = 0$, *i.e.*, the singularity is in the interior of the integration domain and affects all variables. We will now give a sequence of transformations which yields an integrand $\tilde{g}(\zeta)$ which is only singular with respect to ζ_1 at $\zeta_1 = 0$. We will state the Gevrey regularity of the integrand after each transformation, but we postpone the proofs of these claims to Section 4. Section 3.4 will describe the transformations in more detail and describe the resulting quadrature algorithm.

For the presentation, we recall that for $v = (v_1, \ldots, v_m)$ we defined $\sigma_v := 1 - v_1 - \ldots - v_m$.

Step 1: Transform $(x, y) \in S_d \times S_d$ to $(\check{x}, \check{y}, \tilde{x}, \tilde{y}) \in S_{d-k} \times S_{d-k} \times S_k \times S_k$.

We see from (3.12) that $(\hat{x}, \check{x}) \in S_d$ is equivalent to $\check{x} \in S_{d-k}$ and $\hat{x} \in \sigma_{\check{x}} S_k$. Hence we let $\hat{x} = \sigma_{\check{x}} \tilde{x}$ with $\tilde{x} \in S_k$ and obtain for an integral over $x \in S_d$

$$\int_{x \in S_d} f(x) \mathrm{d}x = \int_{\check{x} \in S_{d-k}} \int_{\tilde{x} \in S_k} f\left(\sigma_{\check{x}} \tilde{x}, \check{x}\right) \mathrm{d}\tilde{x}\, \sigma_{\check{x}}^k \mathrm{d}\check{x}.$$

By applying this to (3.31) we obtain

$$I = \int_{\check{x} \in S_{d-k}} \int_{\check{y} \in S_{d-k}} \int_{\tilde{x} \in S_k} \int_{\tilde{y} \in S_k} g_1(\tilde{x}, \tilde{y}, \check{x}, \check{y}) \mathrm{d}\tilde{y}\, \mathrm{d}\tilde{x}\, \mathrm{d}\check{y}\, \mathrm{d}\check{x} \tag{3.32}$$

$$g_1(\tilde{x}, \tilde{y}, \check{x}, \check{y}) := G\left(\sigma_{\check{x}} \tilde{x}, \check{x}, \sigma_{\check{y}} \tilde{y}, \check{y}\right) \sigma_{\check{x}}^k \sigma_{\check{y}}^k,$$

where g_1 is Gevrey smooth unless $\|(\tilde{x} - \tilde{y}, \check{x}, \check{y})\| = 0$.

Step 2: Use $\tilde{z} := \tilde{y} - \tilde{x}$ to transform $(\tilde{x}, \tilde{y}) \in S_k \times S_k$ to $(\tilde{z}, \tilde{x})$ with $\tilde{z} \in A_k$, $\tilde{x} \in E_k(\tilde{z})$.

Then

$$I = \int_{\check{x} \in S_{d-k}} \int_{\check{y} \in S_{d-k}} \int_{\tilde{z} \in A_k} \int_{\tilde{x} \in E_k(\tilde{z})} g_1(\tilde{x}, \tilde{x} + \tilde{z}, \check{x}, \check{y})\, \mathrm{d}\tilde{x}\, \mathrm{d}\tilde{z}\, \mathrm{d}\check{y}\, \mathrm{d}\check{x}. \tag{3.33}$$

Now $g_2(\tilde{z}, \tilde{x}, \check{x}, \check{y}) := g_1(\tilde{x}, \tilde{x} + \tilde{z}, \check{x}, \check{y})$ is Gevrey smooth unless $\|(\tilde{z}, \check{x}, \check{y})\| = 0$. More precisely, we claim that

$$g_2 \in G^{\delta,\alpha}_{\{1,\ldots,k,2k+1,\ldots,2d\}}(\Omega)$$

with $\Omega := \{(\tilde{z}, \tilde{x}) \mid \tilde{z} \in A_k,\ \tilde{x} \in E_k(\tilde{z})\} \times S_{d-k} \times S_{d-k}$.

We then apply (3.30) to split A_k into $2^{k+1} - 2$ pyramids $A^{\sigma}_{N,M\setminus N}$: With $M = \{1, \ldots, k\}$ we obtain an integral over

$$(\check{x}, \check{y}, \tilde{z}, \tilde{x}) \in S_{d-k} \times S_{d-k} \times \Omega = S_{d-k} \times S_{d-k} \times \bigcup_{N \subset M} \bigcup_{\sigma \in \{-,+\}} \{(\tilde{z}, \tilde{x}) \mid \tilde{z} \in A^{\sigma}_{N,M\setminus N},\ \tilde{x} \in E^{\sigma}_{N,M\setminus N}(\tilde{z})\}.$$

Now

$$D^{N,\sigma} := S_{d-k} \times S_{d-k} \times A^{\sigma}_{N,M\setminus N} \tag{3.34}$$

is a Cartesian product of m pyramids, with $m = 3$ for $1 \le k \le d-1$, $m = 2$ for $k = 0$ and $m = 1$ for $k = d$. By Proposition 3.5 we can split $D^{N,\sigma}$ into m pyramids $D_i^{N,\sigma}$ with base $B_i^{N,\sigma}$, $i = 1, \ldots, m$, yielding an integral over

$$(\check{x}, \check{y}, \tilde{z}, \tilde{x}) \in S_{d-k} \times S_{d-k} \times \Omega = \bigcup_{i=1}^{m} \bigcup_{N \subset M} \bigcup_{\sigma \in \{-,+\}} \{(\check{x}, \check{y}, \tilde{z}, \tilde{x}) \mid (\check{x}, \check{y}, \tilde{z}) \in D_i^{N,\sigma},\ \tilde{x} \in E^{\sigma}_{N,M\setminus N}(\tilde{z})\}.$$

Note that by (3.27), (3.28) $E^{\sigma}_{N,M\setminus N}(\tilde{z})$ is an affine image of S_k, and we can parameterize it with $\tilde{X} \in S_k$.

Step 3: For $w = (\check{x}, \check{y}, \tilde{z}) \in D_i^{N,\sigma}$ use $w = s \cdot u$ with $(s, u) \in [0, 1] \times B_i^{N,\sigma}$.

We have $D_i^{N,\sigma} \subset \mathbb{R}^{\tilde{d}}$ with $\tilde{d} = k + 2(d-k) = 2d - k$. Note that the parameter $s \in [0, 1]$ satisfies $s \sim \|w\|$, and that the determinant of the Jacobian gives a factor of $s^{\tilde{d}-1} = s^{2d-k-1}$. We claim that the resulting integrands $g_3^{N,\sigma,i}(s, u)$ satisfy

$$g_3^{N,\sigma,i} \in G^{\delta,\tilde{\alpha}}_{\{1\}}(\Omega_3) \tag{3.35}$$

with $\Omega_3 = \{(s, \check{X}, \check{Y}, \tilde{Z}, \tilde{x}) \mid s \in [0, 1],\ (\check{X}, \check{Y}, \tilde{Z}) \in B_i^{N,\sigma},\ \tilde{x} \in E^{\sigma}_{N,M\setminus N}(s\tilde{Z})\}$ and $\tilde{\alpha} = \alpha + 2d - k - 1$.

TABLE 1. Number K of integrals after transformation in (3.37).

d	$k=0$	$k=1$	$k=2$	$k=3$	$k=4$
1	2	2			
2	2	6	6		
3	2	6	18	14	
4	2	6	18	42	30

Now we parameterize $u \in B_i^{N,\sigma}$ using $S_j \times S_{k-j-1} \times S_{d-k} \times S_{d-k}$ or $[0,1] \times S_j \times S_{k-j-1} \times S_{d-k-1} \times S_{d-k}$ using affine mappings: The pyramid $D_i^{N,\sigma} \subset \mathbb{R}^{\tilde{d}}$ has a $(\tilde{d}-1)$-dimensional base $B_i^{N,\sigma} \subset \mathbb{R}^{\tilde{d}}$. In (3.24) the base $B^+_{N,M\setminus N}$ of $A^+_{N,M\setminus N}$ is expressed with $S_{\#N} \times B_{\#(M\setminus N)}$. By (3.34), (3.19) we have for $1 \le k \le d-1$ with $m=3$

$$B_1^{N,+} = B_{d-k} \times S_{d-k} \times P(B^+_{N,M\setminus N}), \qquad B_2^{N,+} = S_{d-k} \times B_{d-k} \times P(B^+_{N,M\setminus N}), \qquad B_3^{N,+} = S_{d-k} \times S_{d-k} \times B^+_{N,M\setminus N}.$$

Let $j = \#N$, then we parameterize $B^+_{N,M\setminus N}$ with $S_j \times B_{k-j}$ and $P(B^+_{N,M\setminus N})$ with $[0,1] \times S_j \times B_{k-j}$. Finally we use (3.15) to parameterize B_i with S_{i-1}. As we used affine mappings for the parameterization of u we claim that we obtain the same Gevrey regularity as (3.35) on the new domain. Corresponding arguments apply for $A^-_{N,M\setminus N}$, and for the cases $k=0$, $k=d$.

Step 4. Use (3.12) to parameterize all simplices S_p by $[0,1]^p$.

We therefore obtain with $\zeta_1 = s$

$$I = \sum_{N \subset M} \sum_{\sigma \in \{-,+\}} \sum_{j=1}^{3} \int_{\zeta \in [0,1]^{2d}} \tilde{g}_{N,\sigma,j}(\zeta) \mathrm{d}\zeta. \tag{3.36}$$

We claim that we have Gevrey regularity

$$\tilde{g}_{N,\sigma,m} \in G^{\delta,\tilde{\alpha}}_{\{1\}}([0,1]^{2d})$$

since the parameterization only affected the "smooth variables" with numbers $2, \dots, 2d$.

In the case $1 \le k \le d-1$ we have in (3.34) $m=3$ nontrivial factors, and we obtain for the integral a sum of $K = 3(2^{k+1}-2)$ terms.

In the case $k=0$ there are no variables $\tilde{z}, \tilde{x}$ and there is no splitting of A_d, and nothing to do in Step 2. In (3.34) we have $D^{N,\sigma} = S_{d-k} \times S_{d-k}$, *i.e.*, $m=2$ nontrivial factors. Hence we obtain for the integral a sum of $K=2$ terms.

In the case $k=d$ equation (3.34) becomes $D^{N,\sigma} = A^{\sigma}_{N,M\setminus N}$, *i.e.*, we have $m=1$. We obtain for the integral a sum of $K = 2^{k+1}-2$ terms.

To summarize: The total number K of terms in the sum for the integral is

$$K = \begin{cases} 2 & \text{for } k=0 \\ 3(2^{k+1}-2) & \text{for } 1 \le k \le d-1 \\ 2^{k+1}-2 & \text{for } k=d. \end{cases} \tag{3.37}$$

Table 1 shows the number K for $d = 1, \dots, 4$.

3.4. **Detailed form of transformed integrals**

Here we want to give the resulting integrals explicitly as nested one-dimensional integrals

$$\int_{\xi_1=a_1}^{b_1}\int_{\xi_2=a_2(\xi_1)}^{b_2(\xi_1)}\cdots\int_{\xi_{2d}=a_{2d}(\xi_1,\ldots,\xi_{2d-1})}^{b_{2d}(\xi_1,\ldots,\xi_{2d-1})}\tilde{g}_0(\xi)\mathrm{d}\xi.$$

Then we can introduce the variables $\zeta_1,\ldots,\zeta_{2d}$ with $\xi_j = a_j(\xi_1,\ldots,\xi_{j-1})+(b_j(\xi_1,\ldots,\xi_{j-1})-a_j(\xi_1,\ldots,\xi_{j-1}))\,\zeta_j$ and obtain integrals in the form (3.36).

In Step 1 we have

$$g_1(\tilde{x},\tilde{y},\check{x},\check{y}) := G(\sigma_{\check{x}}\tilde{x},\check{x},\sigma_{\check{y}}\tilde{y},\check{y})\sigma^k_{\check{x}}\sigma^k_{\check{y}}. \tag{3.38}$$

In Step 2 we obtain $I=\sum_{N\subset M}\sum_{\sigma\in\{-,+\}} I^{\sigma}_{N,M\setminus N}$ with

$$I^{\sigma}_{N,M\setminus N} = \int_{\check{x}\in S_{d-k}}\int_{\check{y}\in S_{d-k}}\int_{\tilde{z}\in A^{\sigma}_{N,M\setminus N}}\int_{\tilde{x}\in E^{\sigma}_{N,M\setminus N}(\tilde{z})} g_1(\tilde{x},\tilde{x}+\tilde{z},\check{x},\check{y})\,\mathrm{d}\tilde{x}\,\mathrm{d}\tilde{z}\,\mathrm{d}\check{y}\,\mathrm{d}\check{x}.$$

Note that $A^-_{N^-,N^+} = -A^+_{N^+,N^-}$ and $E^-_{N^-,N^+}(-\tilde{z}) = \tilde{z}+E^+_{N^+,N^-}(\tilde{z})$. Hence we have

$$I_{N,M\setminus N} := I^+_{N,M\setminus N} + I^-_{M\setminus N,M} = \int_{\check{x}\in S_{d-k}}\int_{\check{y}\in S_{d-k}}\int_{\tilde{z}\in A^+_{N,M\setminus N}}\int_{\tilde{x}\in E^+_{N,M\setminus N}(\tilde{z})} f(\tilde{z},\tilde{x},\check{x},\check{y})\,\mathrm{d}\tilde{x}\,\mathrm{d}\tilde{z}\,\mathrm{d}\check{y}\,\mathrm{d}\check{x}$$

with

$$f(\tilde{z},\tilde{x},\check{x},\check{y}) := g_1(\tilde{x},\tilde{x}+\tilde{z},\check{x},\check{y}) + g_1(\tilde{x}+\tilde{z},\tilde{x},\check{x},\check{y}). \tag{3.39}$$

For strongly elliptic boundary integral equations resulting from boundary reduction of second order elliptic boundary value problems, the strongest singularity in the integrand is antisymmetric as a function of z and therefore eliminated in the function f, *cf.* [8], Chapter 7, [11], [19], Chapter 5.

Next we can group all sets N with the same number j of elements together and obtain with $N_j=\{1,\ldots,j\}$, $N_0=\{\}$, $R_j = M\setminus N_j = \{j+1,\ldots,k\}$ that

$$I = I_0 + \ldots + I_{k-1} \tag{3.40}$$

where

$$I_j = \int_{\check{x}\in S_{d-k}}\int_{\check{y}\in S_{d-k}}\int_{\tilde{z}\in A^+_{N_j,R_j}}\int_{\tilde{x}\in E^+_{N_j,R_j}(\tilde{z})} f_j(\tilde{z},\tilde{x},\check{x},\check{y})\,\mathrm{d}\tilde{x}\,\mathrm{d}\tilde{z}\,\mathrm{d}\check{y}\,\mathrm{d}\check{x}$$

and f_j is a sum of $\binom{k}{j}$ terms: For $N\subset M$ and a vector $v\in\mathbb{R}^k$ we define the permutation $w=P_N v$ by $w_N=(v_1,\ldots,v_j)$ and $w_{M\setminus N}=(v_{j+1},\ldots,v_k)$ with $j=\#N$. Then

$$f_j(\tilde{z},\tilde{x},\check{x},\check{y}) := \sum_{\substack{N\subset M\\ \#N=j}} f(P_N\tilde{z},P_N\tilde{x},\check{x},\check{y}). \tag{3.41}$$

Using the definition of $E^+_{N_j,R_j}(\tilde{z})$ we define

$$h_j(\tilde{z},\check{x},\check{y}) := \int_{\tilde{x}\in E^+_{N_j,R_j}(\tilde{z})} f_j(\tilde{z},\tilde{x},\check{x},\check{y})\mathrm{d}\tilde{x} = \int_{\tilde{x}\in S_k} f_j(\tilde{z},-\tilde{z}^{(N_j)}+\sigma_{\tilde{z}_{R_j}}\tilde{x},\check{x},\check{y})\sigma^k_{\tilde{z}_{R_j}}\,\mathrm{d}\tilde{x} \tag{3.42}$$

and have

$$I_j = \int_{\check{x}\in S_{d-k}}\int_{\check{y}\in S_{d-k}}\int_{\tilde{z}\in A^+_{N_j,R_j}} h_j(\tilde{z},\check{x},\check{y})\,\mathrm{d}\tilde{z}\,\mathrm{d}\check{y}\,\mathrm{d}\check{x}.$$

Note that the integration domain $S_{d-k} \times S_{d-k} \times A^+_{N_j,R_j}$ is a Cartesian product of pyramids, but S_{d-k} is empty for $d = k$ (no $\check{x}, \check{y}$ variables), and $A^+_{N_j,R_j}$ is empty for $k = 0$ (no $\tilde{z}$ variable). Therefore I_j is an integral over the domain

$$D_j := \begin{cases} S_{d-k} \times S_{d-k} & \text{for } k = 0 \\ S_{d-k} \times S_{d-k} \times A^+_{N_j,R_j} & \text{for } 1 \le k \le d-1 \\ A^+_{N_j,R_j} & \text{for } k = d. \end{cases}$$

We then use that the domain D_j is a Cartesian product of m pyramids, with $m = 1$ for $k = d$, $m = 2$ for $k = 0$, $m = 3$ for $1 \le k \le d-1$ and can therefore be divided into m pyramids, yielding a sum of m terms for I_j.

In Step 3 we parameterize the m integrals for I_j in terms of $[0,1]$ or S_ℓ.

For the integrals over $\check{x} \in S_{d-k}$ and $\check{y} \in S_{d-k}$ we use (3.16) with outer variables s_1, s_2 respectively. By (3.25) $A^+_{N,M\setminus N}$ is a pyramid where the base is a Cartesian product of $-S_{\#N}$ and $B_{\#(M\setminus N)}$. Therefore we can apply (3.17) and obtain a nested integral with outer variable s_3 and inner variables $\tilde{z}_N$, $(\tilde{z}_{M\setminus N})'$.

Case $1 \le k \le d-1$: We get

$$I_j = \int_{s_1=0}^1 \int_{s_2=0}^1 \int_{s_3=0}^1 (s_1 s_2)^{d-k-1} s_3^{k-1} G_j(s_1, s_2, s_3) \mathrm{d}s_3 \mathrm{d}s_2 \mathrm{d}s_1 \tag{3.43}$$

$$\begin{aligned} G_j(s_1, s_2, s_3) := \int_{\check{x}' \in S_{d-k-1}} \int_{\check{y}' \in S_{d-k-1}} \int_{\tilde{z}_{N_j} \in S_j} \int_{\tilde{z}'_{R_j} \in S_{k-j-1}} h_j \\ \times \left(s_3(-\tilde{z}_{N_j}, \tilde{z}'_{R_j}, \sigma_{\tilde{z}'_{R_j}}), s_1(\check{x}', \sigma_{\check{x}'}), s_2(\check{y}', \sigma_{\check{y}'}) \right) \mathrm{d}\tilde{z}'_{R_j} \mathrm{d}\tilde{z}_{N_j} \mathrm{d}\check{y}' \mathrm{d}\check{x}' \end{aligned} \tag{3.44}$$

where expressions of the type $\tilde{z}'_N$ mean $(\tilde{z}_N)'$.

We use

$$\int_{s_1=0}^1 \int_{s_2=0}^1 \int_{s_3=0}^1 G(s_1, s_2, s_3) \mathrm{d}s_3 \mathrm{d}s_2 \mathrm{d}s_1 = \int_{s=0}^1 s^2 \int_{t=0}^1 \int_{u=0}^1 \left(G(s, st, su) + G(st, s, su) + G(st, su, s) \right) \mathrm{d}u \, \mathrm{d}t \, \mathrm{d}s$$

to split (3.43) into $m = 3$ terms as follows:

$$I_j = \int_{s=0}^1 s^{2d-k-1} F_j(s) \mathrm{d}s \tag{3.45}$$

$$F_j(s) := \int_{t=0}^1 t^{d-k-1} \int_{u=0}^1 \left(u^{k-1} G_j(s, st, su) + u^{k-1} G_j(st, s, su) + u^{d-k-1} G_j(st, su, s) \right) \mathrm{d}u \, \mathrm{d}t. \tag{3.46}$$

Case $k = 0$: Here we let $I = I_0$ and have instead of (3.43)

$$I_0 = \int_{s_1=0}^1 \int_{s_2=0}^1 (s_1 s_2)^{d-k-1} G_0(s_1, s_2) \mathrm{d}s_2 \mathrm{d}s_1 \tag{3.47}$$

$$G_0(s_1, s_2) := \int_{\check{x}' \in S_{d-k-1}} \int_{\check{y}' \in S_{d-k-1}} h_0 \left(s_1(\check{x}', \sigma_{\check{x}'}), s_2(\check{y}', \sigma_{\check{y}'}) \right) \mathrm{d}\check{y}' \mathrm{d}\check{x}'. \tag{3.48}$$

With

$$\int_{s_1=0}^1 \int_{s_2=0}^1 G(s_1, s_2) \mathrm{d}s_2 \mathrm{d}s_1 = \int_{s=0}^1 s \left(\int_{t=0}^1 G(s, st) \mathrm{d}t + \int_{t=0}^1 G(st, s) \mathrm{d}t \right) \mathrm{d}s$$

we split (3.47) into $m = 2$ terms to obtain (3.45) with

$$F_0(s) := \int_{t=0}^{1} t^{d-1} \left(G_0(s, st) + G_0(st, s)\right) \mathrm{d}t. \tag{3.49}$$

As there are no $\tilde{z}, \tilde{x}$-variables, we have instead of (3.42) simply

$$h_0(\check{x}, \check{y}) = g_1(\check{x}, \check{y}). \tag{3.50}$$

Case $k = d$: Here $m = 1$ and we have instead of (3.43)

$$I_j = \int_{s_3=0}^{1} s_3^{k-1} G_j(s_3) \mathrm{d}s_3 \tag{3.51}$$

$$G_j(s_3) := \int_{\tilde{z}_{N_j} \in -S_j} \int_{\tilde{z}'_{R_j} \in S_{k-j-1}} h_j \left(s_3 \tilde{z}_{N_j}, s_3(\tilde{z}'_{R_j}, \sigma_{\tilde{z}'_{R_j}})\right) \mathrm{d}\tilde{z}'_{R_j} \mathrm{d}\tilde{z}_{N_j}. \tag{3.52}$$

In this case we obtain (3.45) with

$$F_j(s) := G_j(s). \tag{3.53}$$

For our quadrature algorithm we will use composite Gauss quadrature $Q_{n,m}$ with $m = O(n^{1/\delta})$ for the outermost variable s, and standard Gaussian quadrature Q_n for all inner variables.

Remark 3.7. If we implement this algorithm directly in machine arithmetic there will be function evaluations $G(x, y)$ with $\|x - y\| \approx \sigma^m \ll 1$ which will lead to subtractive cancellation if σ^m is of the order of the machine epsilon or less. To avoid subtractive cancellation, we should use $G(x, y) = H(x, y, \hat{y} - \hat{x}, \check{x}, \check{y})$ and evaluate H instead of G: note that we have for given $\check{x}, \check{y}, \tilde{z}, \tilde{x}$

$$\hat{z} = \hat{y} - \hat{x} = \sigma_{\check{y}}(\tilde{x} + \tilde{z}) - \sigma_{\check{x}}\tilde{x} = \sigma_{\check{y}}\tilde{z} + (\textstyle\sum_j \check{x}_j - \sum_j \check{y}_j)\tilde{x}.$$

We use instead of (3.38) the function $g_2(\tilde{z}, \tilde{x}, \check{x}, \check{y}) = g_1(\tilde{x}, \tilde{x} + \tilde{z}, \check{x}, \check{y})$ and evaluate it in terms of H as

$$g_2(\tilde{z}, \tilde{x}, \check{x}, \check{y}) := H\left((\sigma_{\check{x}}\tilde{x}, \check{x}),\ (\sigma_{\check{y}}(\tilde{x} + \tilde{z}), \check{y}),\ \sigma_{\check{y}}\tilde{z} + (\textstyle\sum_j \check{x}_j - \sum_j \check{y}_j)\tilde{x},\ \check{x},\ \check{y}\right) \sigma_{\check{x}}^k \sigma_{\check{y}}^k. \tag{3.54}$$

We replace (3.39) with

$$f(\tilde{z}, \tilde{x}, \check{x}, \check{y}) := g_2(\tilde{z}, \tilde{x}, \check{x}, \check{y}) + g_2(-\tilde{z}, \tilde{x} + \tilde{z}, \check{x}, \check{y}). \tag{3.55}$$

We now summarize the resulting quadrature algorithm:

- Sum over $j = 0, \ldots, \max\{0, k-1\}$ in (3.40);
- Composite Gauss quadrature for $s \in [0, 1]$ in (3.45);
- $\begin{cases} \text{If } 1 \le k \le d-1: & \text{Gauss quadrature for } (t, u) \in [0,1]^2 \text{ in (3.46)} \\ \text{if } k = 0: & \text{Gauss quadrature for } t \in [0,1] \text{ in (3.49)} \\ \text{if } k = d: & F_j \text{ given by (3.53)}; \end{cases}$
- If $k \le d-1$: Gauss quadrature for $(\check{x}', \check{y}') \in S_{d-k-1} \times S_{d-k-1}$ in (3.44), (3.48);
- If $k \ge 1$:
  - Gauss quadrature for $(\tilde{z}_{N_j}, \tilde{z}'_{R_j}) \in S_j \times S_{k-j-1}$ in (3.44), (3.52),
  - Gauss quadrature for $\tilde{x} \in S_k$ in (3.42),
  - sum over all j-element subsets N of $\{1, \ldots k\}$ in (3.41), sum in (3.55).

  If $k = 0$: $h_0(\check{x}, \check{y}) := g_2(\check{x}, \check{y})$;
- g_2 is defined in terms of H by (3.54).

We can now count the number of quadrature points: For the integral over $s \in [0,1]$ we use composite Gauss quadrature $Q_{n,m}$ with $m = Cn^{1/\delta}$ subintervals, see Definition 2.4. Note that we can either have the constant order rule $Q_{n,m} = Q_{n,m,\sigma}$, or the variable order rule $Q_{n,m} = Q_{n,m,\sigma,\delta}$. In both cases we obtain $N_1 = O(nm) = O(n^{1+1/\delta})$ quadrature points for the integral over s. For the remaining $2d-1$ directions we use Gauss quadrature Q_n with n quadrature nodes. Since have a sum of K terms with K given by (3.37) the total number of quadrature points is

$$N = KN_1 n^{2d-1} = KCn^{2d+1/\delta}. \tag{3.56}$$

Note that it is also possible to use for the singular integration a value $\tilde{n} = cn$ instead of n, see the numerical experiments in Section 6.

4. Gevrey regularity under coordinate transformations and convergence of quadrature

4.1. Preliminaries

In the previous section we performed a series of transformations and obtained

$$I = \int_{x\in S_d} \int_{y\in S_d} G(x,y)\,\mathrm{d}y\mathrm{d}x = \int_{\zeta\in[0,1]^{2d}} \tilde{g}(\zeta)\,\mathrm{d}\zeta \tag{4.1}$$

with

$$\tilde{g}(\zeta) := \sum_{N\subset M} \sum_{\sigma\in\{-,+\}} \sum_{j=1}^{m} \tilde{g}_{N,\sigma,j}(\zeta). \tag{4.2}$$

The main result of this section is given by Theorem 4.5. It shows that under suitable assumptions on the integrand G, the quadrature rule of tensor product type is applicable to the transformed function $\tilde{g}$ and converges exponentially fast to the exact value I of the integral.

The section is organized as follows. In Section 4.2 we formulate Theorem 4.2, which gives the necessary regularity properties of the transformed function $\tilde{g}$. Then Theorem 4.5 is a corollary of Theorem 4.2 and Proposition 2.8. In Section 4.3 we prove Theorem 4.2 and auxiliary Lemmas 4.7–4.10. Section 4.4 contains two technical lemmas required in the proof of Lemma 4.7.

4.2. Main result

As in the previous section we split $x = (\hat{x}, \check{x})$ with $\hat{x} := (x_1, \dots, x_k)$, $\check{x} := (x_{k+1}, \dots, x_n)$ and similarly $y = (\hat{y}, \check{y})$. We make

Assumption 4.1. *Let $k \in \{0, \dots, d\}$, $\delta \geq 1$, $\alpha > k - 2d$ and assume $G(x,y) = H(x, y, \hat{y} - \hat{x}, \hat{x}, \hat{y})$ with*

$$H(x,y,\xi,\eta,\zeta) \in G^{\delta,\alpha}_{\{2d+1,\dots,4d-k\}}(\Omega') \quad \textit{where} \quad \Omega' := S_d \times S_d \times (S_k - S_k) \times S_{d-k} \times S_{d-k}, \tag{4.3}$$

i.e. $\exists\, A_0, A_1 > 0$ *independent of* $\nu := (\nu^\circ, \nu^*) \in \mathbb{N}_0^{2d} \times \mathbb{N}_0^{2d-k}$ *and* $(x,y,\xi,\eta,\zeta) \in \Omega'$ *such that*

$$|D^{\nu^\circ}_{(x,y)} D^{\nu^*}_{(\xi,\eta,\zeta)} H(x,y,\xi,\eta,\zeta)| \leq A_0 A_1^{|\nu|} (\nu!)^\delta \|(\xi,\eta,\zeta)\|^{\min(\alpha - |\nu^*|, 0)}. \tag{4.4}$$

Note that Assumption 4.1 is satisfied if the integral I is defined by (3.1) where (i) the simplices $S^{(1)}$ and $S^{(2)}$ satisfy Assumption 3.1 and (ii) the function $g(x,y)$ in (3.1) satisfies Assumption 3.2. Then the function $G(u,v)$ in (3.4), (3.5) satisfies (3.11) and therefore Assumption 4.1.

Theorem 4.2. *Suppose G satisfies Assumption 4.1 and $\tilde{g}$ is obtained from G by the sequence of the coordinate transformations given by Steps 1–3 from the previous section. Then*

$$\tilde{g}(\zeta) \in G^{\delta,\tilde{\alpha}}_{\{1\}}([0,1]^{2d}) \quad \text{with} \quad \tilde{\alpha} = \alpha + 2d - k - 1. \tag{4.5}$$

Remark 4.3. Theorem 4.2 shows that the transformations in Section 3.3 isolate the singularity of the integrand $\tilde{g}(\zeta)$ in the coordinate direction ζ_1, while preserving Gevrey regularity in the remaining coordinates. We remark that in certain special cases when α is an integer (such as, *e.g.*, in boundary integral equations stemming from boundary reduction of second order elliptic boundary value problems), these transformations actually completely *remove* the singularity. In this case, the assertion (4.5) of Theorem 4.2 can be strengthened to $\tilde{g} \in G^{\delta}([0,1]^{2d})$ (generalizing the case $d = 3$ and $\alpha = -1, -2$ in [19], Chap. 5).

The proof of Theorem 4.2 requires auxiliary Lemmas 4.7–4.10 and is given at the end of the section. Theorem 4.2 allows an explicit construction of a quadrature rule for G on $S_d \times S_d$, if G satisfies Assumption 4.1.

Definition 4.4. Let $\hat{Q}^{k,d}_{n,m}$ be the quadrature rule on $S_d \times S_d$ such that

$$\hat{Q}^{k,d}_{n,m} G = [Q_{n,m} \otimes \underbrace{Q_n \otimes \cdots \otimes Q_n}_{2d-1 \text{ times}}]\tilde{g} \tag{4.6}$$

where $Q_{n,m}$ is the quadrature rule in Definition 2.4, and $\tilde{g}$ is given in (4.2). Note that $Q_{n,m}$ can be either the constant order composite rule $Q_{n,m,\sigma}$ with $\sigma \in (0,1)$, or the variable order composite rule $Q_{n,m,\sigma,\delta}$ with $\sigma \in (0,1)$ and $\delta \geq 1$.

Theorem 4.5. *Suppose G satisfies Assumption 4.1. Let $b > 0$ and $m = \lceil bn^{1/\delta} \rceil$. Then there exist $r, r', C > 0$ so that for all $n \in \mathbb{N}$*

$$\left| \int_{x \in S_d} \int_{y \in S_d} g(x,y)\,\mathrm{d}x\mathrm{d}y - \hat{Q}^{k,d}_{n,m} g \right| \leq C \exp(-rn^{1/\delta}) = C \exp(-r' N^{1/(2d\delta+1)}) \tag{4.7}$$

where $N = O(n^{2d+1/\delta})$ is the number of function evaluations in the quadrature rule $\hat{Q}^{k,d}_{n,m}$.

Proof. The assertion of the theorem follows directly from Theorem 4.2 and Proposition 2.8. □

Remark 4.6. The quadrature rule $\hat{Q}^{k,d}_{n,m}$ given by (4.6) is $2d$-fold tensor products rule applied to $\tilde{g}(\zeta)$. Since $\tilde{g}(\zeta)$ is singular in ζ_1 and smooth in the remaining coordinates, the rule uses the composite Gauss rule $Q_{n,m}$ in ζ_1 and the standard Gauss rule Q_n in the coordinates $\zeta_2, \ldots, \zeta_{2d}$. In the special case mentioned in Remark 4.3 the integrand $\tilde{g}$ is smooth in *all* coordinates $\zeta_1, \ldots, \zeta_{2d}$. Hence we can use instead of 4.6 the rule $\hat{Q}^{k,d}_{n,m} G := [Q_n \otimes \cdots \otimes Q_n]\tilde{g}$ which uses standard Gauss quadrature for $\zeta_1, \ldots, \zeta_{2d}$. Then Remark 2.9 gives in place of (4.7) the convergence rate

$$\left| \int_{x \in S_d} \int_{y \in S_d} g(x,y)\,\mathrm{d}x\mathrm{d}y - \hat{Q}^{k,d}_{n,m} g \right| \leq C \exp(-rn^{1/\delta}) = C \exp(-r' N^{1/(2d\delta)}). \tag{4.8}$$

4.3. Proof of the main result

We give the proof of Theorem 4.2. To this end, we set up some notation and then verify preservation of Gevrey regularity under composition by establishing bounds on the growth of derivatives in three technical lemmas. We recall $\sigma_{\check{x}} = 1 - \sum_j \check{x}_j$, $\sigma_{\check{y}} = 1 - \sum_j \check{y}_j$,

$$g_1(\tilde{x}, \tilde{y}, \check{x}, \check{y}) := G(\sigma_{\check{x}}\tilde{x}, \check{x}, \sigma_{\check{y}}\tilde{y}, \check{y})\sigma^k_{\check{x}}\sigma^k_{\check{y}} \tag{4.9}$$

and

$$g_2(\tilde{z}, \tilde{x}, \check{x}, \check{y}) := g_1(\tilde{x}, \tilde{x} + \tilde{z}, \check{x}, \check{y}). \tag{4.10}$$

Assumption 4.1, (4.9) and (4.10) give

$$g_2(\tilde{z},\tilde{x},\check{x},\check{y}) := (H\circ\phi)(\tilde{z},\tilde{x},\check{x},\check{y})\sigma_{\tilde{x}}^k\sigma_{\check{y}}^k, \quad \text{with} \quad \phi(\tilde{z},\tilde{x},\check{x},\check{y}) = (\sigma_{\check{x}}\tilde{x},\check{x},\sigma_{\check{y}}(\tilde{x}+\tilde{z}),\check{y},\sigma_{\check{y}}(\tilde{x}+\tilde{z})-\sigma_{\check{x}}\tilde{x},\check{x},\check{y}). \tag{4.11}$$

Lemma 4.7. *Suppose H satisfies (4.4) and g_2, ϕ are given by (4.11). Then*

$$g_2(\tilde{z},\tilde{x},\check{x},\check{y}) \in G^{\delta,\alpha}_{\{1,\ldots,k,2k+1,\ldots 2d\}}(\Omega), \quad \textit{with} \quad \Omega = \{(\tilde{z},\tilde{x}) \mid \tilde{z}\in A_k,\ \tilde{x}\in E_k(\tilde{z})\}\times S_{d-k}\times S_{d-k}, \tag{4.12}$$

i.e. $\exists\, C_0, C_1 > 0$ *independent of* $\nu = (\nu^\circ,\nu^*) \in \mathbb{N}_0^k \times \mathbb{N}_0^{2d-k}$ *and* $(\tilde{z},\tilde{x},\check{x},\check{y}) \in \Omega$ *such that*

$$|D_{\tilde{x}}^{\nu^\circ} D^{\nu^*}_{(\tilde{z},\check{x},\check{y})} g_2(\tilde{z},\tilde{x},\check{x},\check{y})| \le C_0 C_1^{|\nu|}(\nu!)^\delta \|(\tilde{z},\check{x},\check{y})\|^{\min(\alpha-|\nu^*|,0)}. \tag{4.13}$$

Proof. First we prove that the function $H\circ\phi$ satisfy the estimate (4.26) and then generalize this result for g_2. Recalling (4.3) and (4.9)–(4.11) we have $\Omega\subset\mathbb{R}^{2d}$, $\Omega'\subset\mathbb{R}^{4d-k}$, $\phi:\Omega\to\Omega'$ is a polynomial (4.11) and $H:\Omega'\to\mathbb{R}$ is of class C^∞ *in the interior of* Ω'. Define $s := (\tilde{z},\tilde{x},\check{x},\check{y}) \in \Omega$ and $t := \phi(s) \in \Omega'$. We recall a multivariate version of the formula of Faà di Bruno [3], which represents the chain rule for multivariate composite functions

$$D_s^\nu(H\circ\phi)(s) = \sum_{l=1}^{|\nu|} \sum_{\begin{pmatrix} j_1,\ldots,j_l \\ \beta_{(1)},\ldots,\beta_{(l)}\end{pmatrix}\in\mathcal{M}_{\nu,l}} \gamma^{|\nu|,n,l}_{j,\beta_{(1)},\ldots,\beta_{(l)}} (D^l_{t_{j_1}\ldots t_{j_l}} H(t)) \prod_{i=1}^{l} (D_s^{\beta_{(i)}}\phi_{j_i}(s)). \tag{4.14}$$

Here $\gamma^{|\nu|,2d,l}_{j,\beta_{(1)},\ldots,\beta_{(l)}}$ are positive integers and the sum is taken over the set

$$\mathcal{M}_{\nu,l} := \left\{ \begin{pmatrix} j_1,\ldots,j_l \\ \beta_{(1)},\ldots,\beta_{(l)}\end{pmatrix} : j_1,\ldots,j_l\in\{1,\ldots,4d-k\} \text{ and } \beta_{(1)}+\ldots+\beta_{(l)} = \nu \text{ and } \beta_{(i)}\neq 0,\ i=1,\ldots,l \right\}. \tag{4.15}$$

Note that $j_1,\ldots,j_l\in\mathbb{N}$ are integers and $\beta_{(1)},\ldots,\beta_{(l)}\in\mathbb{N}^{2d}$ are multiindices of the same length as ν, *i.e.* $2d$. Let us consider the multiindex ν and the associated differential operator D_s^ν. By grouping the derivatives w.r.t. $\tilde{x}$ and w.r.t. $(\tilde{z},\check{x},\check{y})$ in ν we obtain

$$D_s^\nu \equiv D_{\tilde{x}}^{\nu^\circ} D^{\nu^*}_{(\tilde{z},\check{x},\check{y})}, \tag{4.16}$$

which introduces a splitting of $\nu = (\nu^\circ,\nu^*)$. Note that ν° consists of k components, since $\tilde{x}\in\mathbb{R}^k$ and ν^* consists of $2d-k$ components, since $(\tilde{z},\check{x},\check{y})\in\mathbb{R}^{2d-k}$. In the same manner we decompose the multiindices $\beta_{(i)} = (\beta^\circ_{(i)},\beta^*_{(i)})$, $i=1,\ldots,l$ such that

$$D_s^{\beta_{(i)}} \equiv D_{\tilde{x}}^{\beta^\circ_{(i)}} D^{\beta^*_{(i)}}_{(\tilde{z},\check{x},\check{y})}. \tag{4.17}$$

Let us consider every particular summand in (4.14). Assume that the sets $j_1,\ldots,j_l$ and $\beta_{(1)},\ldots,\beta_{(l)}$ are fixed. We group j_i and $\beta_{(i)}$ with the same index i and define

$$\mathcal{N} := \{(j_1,\beta_{(1)}),\ldots,(j_l,\beta_{(l)})\}.$$

In what follows we obtain an upper bound for

$$\left| D^l_{t_{j_1}\ldots t_{j_l}} H(t)\right| \prod_{i=1}^{l} \left| D_s^{\beta_{(i)}}\phi_{j_i}(s)\right|.$$

Let us introduce a disjoint decomposition of the set of pairs $\mathcal{N} = \mathcal{N}_1 \dot\cup \mathcal{N}_2 \dot\cup \mathcal{N}_3$, where

$$\begin{aligned}
\mathcal{N}_1 &:= \big\{(j_i, \beta_{(i)}) \in \mathcal{N} : j_i \in \{1, \dots, 2d\}\big\} \\
\mathcal{N}_2 &:= \big\{(j_i, \beta_{(i)}) \in \mathcal{N} : j_i \in \{2d+1, \dots, 2d+k\}\big\} \\
\mathcal{N}_3 &:= \big\{(j_i, \beta_{(i)}) \in \mathcal{N} : j_i \in \{2d+k+1, \dots, 4d-k\}\big\}
\end{aligned}$$

and let us split $\mathcal{N}_2 = \mathcal{N}_{2,0} \dot\cup \mathcal{N}_{2,1} \dot\cup \mathcal{N}_{2,2}$ and $\mathcal{N}_3 = \mathcal{N}_{3,0} \dot\cup \mathcal{N}_{3,1}$, where

$$\begin{aligned}
\mathcal{N}_{2,0} &:= \big\{(j_i, \beta_{(i)}) \in \mathcal{N}_2 : |\beta^\circ_{(i)}| + |\beta^*_{(i)}| \geq 3 \text{ or } |\beta^\circ_{(i)}| \geq 2\big\}, \\
\mathcal{N}_{2,1} &:= \big\{(j_i, \beta_{(i)}) \in \mathcal{N}_2 : \big(|\beta^\circ_{(i)}| = 0 \text{ and } (|\beta^*_{(i)}| = 1 \text{ or } 2)\big) \text{ or } \big(|\beta^\circ_{(i)}| = 1 \text{ and } |\beta^*_{(i)}| = 1\big)\big\}, \\
\mathcal{N}_{2,2} &:= \big\{(j_i, \beta_{(i)}) \in \mathcal{N}_2 : |\beta^\circ_{(i)}| = 1 \text{ and } |\beta^*_{(i)}| = 0\big\}
\end{aligned}$$

and

$$\begin{aligned}
\mathcal{N}_{3,0} &:= \big\{(j_i, \beta_{(i)}) \in \mathcal{N}_3 : |\beta^\circ_{(i)}| \geq 1 \text{ or } |\beta^*_{(i)}| \geq 2\big\}, \\
\mathcal{N}_{3,1} &:= \big\{(j_i, \beta_{(i)}) \in \mathcal{N}_3 : |\beta^\circ_{(i)}| = 0 \text{ and } |\beta^*_{(i)}| = 1\big\}.
\end{aligned}$$

With the above notations we have

$$\left|D_s^{\beta_{(i)}} \phi_{j_i}(s)\right| \leq \begin{cases} 0, & \text{if } (j_i, \beta_{(i)}) \in \mathcal{N}_{2,0} \dot\cup \mathcal{N}_{3,0} \\ 1, & \text{if } (j_i, \beta_{(i)}) \in \mathcal{N}_1 \dot\cup \mathcal{N}_{2,1} \dot\cup \mathcal{N}_{3,1} \\ |\sigma_{\check y} - \sigma_{\check x}|, & \text{if } (j_i, \beta_{(i)}) \in \mathcal{N}_{2,2}. \end{cases} \tag{4.18}$$

This gives

$$\prod_{i=1}^{l} \left|D_s^{\beta_{(i)}} \phi_{j_i}(s)\right| \leq \begin{cases} 0, & \text{if } \mathcal{N}_{2,0} \dot\cup \mathcal{N}_{3,0} \neq \{\}, \\ \displaystyle\prod_{(j_i,\beta_{(i)}) \in \mathcal{N}_{2,1} \cup \mathcal{N}_{2,2} \cup \mathcal{N}_{3,1}} \left|D_s^{\beta_{(i)}} \phi_{j_i}(s)\right|, & \text{if } \mathcal{N}_{2,0} \dot\cup \mathcal{N}_{3,0} = \{\}. \end{cases} \tag{4.19}$$

Using (4.18) we obtain the upper bound

$$\prod_{(j_i,\beta_{(i)}) \in \mathcal{N}_{2,1} \cup \mathcal{N}_{2,2} \cup \mathcal{N}_{3,1}} \left|D_s^{\beta_{(i)}} \phi_{j_i}(s)\right| \leq \prod_{(j_i,\beta_{(i)}) \in \mathcal{N}_{2,2}} \left|D_s^{\beta_{(i)}} \phi_{j_i}(s)\right| \leq |\sigma_{\check y} - \sigma_{\check x}|^{\#\mathcal{N}_{2,2}}.$$

Note that $|\sigma_{\check y} - \sigma_{\check x}| = |\sum_j \check x_j - \sum_j \check y_j| \leq \check C \|(\check x, \check y)\|$ and thus by (4.19)

$$\prod_{i=1}^{l} \left|D_s^{\beta_{(i)}} \phi_{j_i}(s)\right| \leq \begin{cases} 0, & \text{if } \mathcal{N}_{2,0} \cup \mathcal{N}_{3,0} \neq \{\}, \\ C\|(\check x, \check y)\|^{\#\mathcal{N}_{2,2}}, & \text{if } \mathcal{N}_{2,0} \cup \mathcal{N}_{3,0} = \{\}. \end{cases} \tag{4.20}$$

H satisfies (4.4) by assumption which yields

$$\begin{aligned}
|D^l_{t_{j_1} \dots t_{j_l}} H(t)| &\leq A_0 A_1^l (l!)^\delta \|t_{\{2d+1,\dots,4d-k\}}\|^{\min(\alpha - \#\mathcal{N}_2 - \#\mathcal{N}_3, 0)} \\
&\leq \tilde A_0 \tilde A_1^l (l!)^\delta \|(\tilde z, \check x, \check y)\|^{\min(\alpha - \#\mathcal{N}_2 - \#\mathcal{N}_3, 0)},
\end{aligned} \tag{4.21}$$

since $\|t_{\{2d+1,\ldots,4d-k\}}\| \equiv \|(\sigma_{\check{y}}(\tilde{x}+\tilde{z}) - \sigma_{\check{x}}\tilde{x}, \check{x}, \check{y})\| \sim \|(\tilde{z}, \check{x}, \check{y})\|$ by Lemma 4.12. Combining (4.20) and (4.21) we obtain

$$\begin{aligned}\left|D^l_{t_{j_1}\ldots t_{j_l}} H(t)\right| \prod_{i=1}^{l} \left|D_s^{\beta_{(i)}} \phi_{j_i}(s)\right| &\le \tilde{A}_0 \tilde{A}_1^l (l!)^\delta \|(\tilde{z}, \check{x}, \check{y})\|^{\min(\alpha - \#\mathcal{N}_2 - \#\mathcal{N}_3, 0)} \cdot \begin{cases} 0, & \text{if } \mathcal{N}_{2,0} \cup \mathcal{N}_{3,0} \neq \{\} \\ C\|(\check{x}, \check{y})\|^{\#\mathcal{N}_{2,2}}, & \text{if } \mathcal{N}_{2,0} \cup \mathcal{N}_{3,0} = \{\} \end{cases} \\ &\le \tilde{C}_0 \tilde{C}_1^l (l!)^\delta \|(\tilde{z}, \check{x}, \check{y})\|^{\min(\alpha - \#\mathcal{N}_{2,1} - \#\mathcal{N}_{2,2} - \#\mathcal{N}_{3,1}, 0) + \#\mathcal{N}_{2,2}}, \\ &\le C_0 C_1^l (l!)^\delta \|(\tilde{z}, \check{x}, \check{y})\|^{\min(\alpha - \#\mathcal{N}_{2,1} - \#\mathcal{N}_{3,1}, 0)}, \\ &\le C_0 C_1^l (l!)^\delta \|(\tilde{z}, \check{x}, \check{y})\|^{\min(\alpha - |\nu^*|, 0)}. \end{aligned} \tag{4.22}$$

The last inequality holds, since $\|(\tilde{z}, \check{x}, \check{y})\|_\infty \le 1$; $a + \min(b, 0) \ge \min(a+b, 0)$ if $a \ge 0$; $\beta^*_{(1)} + \ldots + \beta^*_{(l)} = \nu^*$ and

$$\#\mathcal{N}_{2,1} + \#\mathcal{N}_{3,1} \le \sum_{(j_i, \beta_{(i)}) \in \mathcal{N}_{2,1} \cup \mathcal{N}_{3,1}} |\beta^*_{(i)}| \le |\nu^*|.$$

We have $l \le |\nu|$ and thus by (4.14) we have

$$\left|D_s^\nu (H \circ \phi)(s)\right| \le C_0 C_1^{|\nu|} (|\nu|!)^{\delta - 1} \|(\tilde{z}, \check{x}, \check{y})\|^{\min(\alpha - |\nu^*|, 0)} \cdot \left(\sum_{l=1}^{|\nu|} \sum_{\left(\begin{smallmatrix} j_1, \ldots, j_l \\ \beta_{(1)}, \ldots, \beta_{(l)} \end{smallmatrix}\right) \in \mathcal{M}_{\nu,l}} \gamma^{|\nu|,n,l}_{j,\beta_{(1)},\ldots,\beta_{(l)}} l! \right). \tag{4.23}$$

In order to estimate the double sum in parentheses we use the identity[4]

$$\sum_{l=1}^{|\nu|} \sum_{\left(\begin{smallmatrix} j_1, \ldots, j_l \\ \beta_{(1)}, \ldots, \beta_{(l)} \end{smallmatrix}\right) \in \mathcal{M}_{\nu,l}} \gamma^{|\nu|,d,l}_{j,\beta_{(1)},\ldots,\beta_{(l)}} l! \prod_{i=1}^{l} |\nu_i|! = 3d(3d+1)^{|\nu|-1} |\nu|!, \tag{4.24}$$

yielding

$$\sum_{l=1}^{|\nu|} \sum_{\left(\begin{smallmatrix} j_1, \ldots, j_l \\ \beta_{(1)}, \ldots, \beta_{(l)} \end{smallmatrix}\right) \in \mathcal{M}_{\nu,l}} \gamma^{|\nu|,d,l}_{j,\beta_{(1)},\ldots,\beta_{(l)}} l! \le (3d+1)^{|\nu|} |\nu|!. \tag{4.25}$$

Inserting in (4.23) and using $|\nu|! \le (2d)^{|\nu|} \nu!$, which holds by the multinomial theorem we obtain

$$\left|D_s^\nu (H \circ \phi)(s)\right| \le \hat{C}_0 \hat{C}_1^{|\nu|} (\nu!)^\delta \|(\tilde{z}, \check{x}, \check{y})\|^{\min(\alpha - |\nu^*|, 0)}. \tag{4.26}$$

The estimate (4.13) follows, since $\sigma_{\check{x}} = 1 - \sum_j \check{x}_j \le 1$, $\sigma_{\check{y}} = 1 - \sum_j \check{y}_j \le 1$ yielding

$$|D_s^\mu \sigma_{\check{x}}^k \sigma_{\check{y}}^k| \le (d!)^2, \qquad \forall \mu \in \mathbb{N}_0^{2d},$$

and thus by the product rule

$$\left|D_s^\nu \big((H \circ \phi)(s) \sigma_{\check{x}}^k \sigma_{\check{y}}^k\big)\right| \le \sum_{\mu \le \nu} \left|D_s^\mu (H \circ \phi)(s)\right| \cdot \left|D_s^{\nu - \mu} (\sigma_{\check{x}}^k \sigma_{\check{y}}^k)\right| \le \max_{\mu \le \nu} \left|D_s^\mu (H \circ \phi)(s)\right| (d!)^2 2^{|\nu|}, \tag{4.27}$$

which together with (4.26) yields the asserted inequality (4.13). □

[4] M. Dauge, personal communication (2007).

Lemma 4.8. *Let $q, q' \in \mathbb{N}$, $\Omega \subset [-1,1]^q$ and $\Omega' \subset [-1,1]^{q'}$. Suppose $N \subset \{1, \dots, \min(q,q')\}$ and $f \in G_N^{\delta,\alpha}(\Omega)$. Let $\Psi : \Omega' \to \Omega$ be a polynomial of degree p such that for $t = \Psi(s)$ there holds $t_N = s_N$. Then*

(i) $\hat{f}(s) := (f \circ \Psi)(s) \in G_N^{\delta,\alpha}(\Omega')$;

(ii) If in addition $q = q'$ and $J_\Psi \neq 0$ in the interior of Ω', then $\tilde{f}(s) := (f \circ \Psi)(s) J_\Psi(s) \in G_N^{\delta,\alpha}(\Omega')$.

Proof. We use the same technique as in the proof of Lemma 4.7. First we prove (i). Recall the formula of Faà Di Bruno (4.14), (4.15) and consider a fixed set $\mathcal{N} := \big\{(j_1, \beta_{(1)}), \dots, (j_l, \beta_{(l)})\big\}$. Define

$$\mathcal{N}_1 := \big\{(j_i, \beta_{(i)}) \in \mathcal{N} : j_i \in N\big\}, \qquad \mathcal{N}_2 = \mathcal{N} \setminus \mathcal{N}_1.$$

Further, define

$$\mathcal{N}_{1,1} := \big\{(j_i, \beta_{(i)}) \in \mathcal{N}_1 : |\beta_{(i)}| = 1, \text{ and } (\beta_{(i)})_{j_i} = 1\big\}, \qquad \mathcal{N}_{1,0} := \mathcal{N} \setminus \mathcal{N}_{1,1}.$$

With the above definitions we have $\mathcal{N} = \mathcal{N}_{1,0} \,\dot\cup\, \mathcal{N}_{1,1} \,\dot\cup\, \mathcal{N}_2$ and

$$\left| D_s^{\beta_{(i)}} \Psi_{j_i}(s) \right| \le \begin{cases} 0, & \text{if } (j_i, \beta_{(i)}) \in \mathcal{N}_{1,0}, \\ 1, & \text{if } (j_i, \beta_{(i)}) \in \mathcal{N}_{1,1}, \\ c(p,q), & \text{if } (j_i, \beta_{(i)}) \in \mathcal{N}_2. \end{cases}$$

Thus

$$\left| D^l_{t_{j_1} \dots t_{j_l}} f(t) \right| \prod_{i=1}^{l} \left| D_s^{\beta_{(i)}} \Psi_{j_i}(s) \right| \le A_0 A_1^l (l!)^\delta \|t_N\|^{\min(\alpha - \#\mathcal{N}_{1,1}, 0)} \le \tilde{A}_0 \tilde{A}_1^l (l!)^\delta \|s_N\|^{\min(\alpha - |\nu_N|, 0)}, \tag{4.28}$$

since $\#\mathcal{N}_{1,1} \le |\nu_N|$. We recall (4.25) and get

$$\left| D_s^\nu (f \circ \Psi)(s) \right| \le C_0 C_1^{|\nu|} (\nu!)^\delta \|s_N\|^{\min(\alpha - |\nu_N|, 0)} \tag{4.29}$$

or $\hat{f} \in G_N^{\delta,\alpha}(\Omega')$. To show (ii) we note that Ψ is a polynomial and $J_\Psi \neq 0$ in the interior of Ω' yield that J_Ψ is a polynomial, thus

$$\exists\, c(p,r) > 0: \quad |D^\mu J_\Psi(s)| \le c(p,r) \quad \forall \mu \in \mathbb{N}_0^r \qquad \forall s \in \Omega'.$$

Hence, by the product rule

$$|D_s^\nu \tilde{f}(s)| \le \sum_{\mu \le \nu} |D_s^\mu (f \circ \Psi)(s)| \cdot |D_s^{\nu - \mu} J_\Psi(s)| \le \tilde{C}_0 \tilde{C}_1^{|\nu|} (\nu!)^\delta \|s_N\|^{\min(\alpha - |\nu_N|, 0)}, \tag{4.30}$$

yielding $\tilde{f} \in G_N^{\delta,\alpha}(\Omega')$. □

Corollary 4.9. *Suppose $f \in G^\delta(S^{(1)} \times S^{(2)})$, where $S^{(1)}, S^{(2)}$ are simplices in $\mathbb{R}^d$. Let $\phi_i : S_d \to S^{(i)}$ be an affine transformation to the reference simplex and $\psi : [0,1]^d \to S_d$ be the parameterization of S_d by simplex coordinates*

$$\psi_1(x) = x_1, \dots, \psi_d(x) = x_d(1 - x_1) \dots (1 - x_{d-1}). \tag{4.31}$$

Define $\Psi := (\phi_1 \circ \psi, \phi_2 \circ \psi) : [0,1]^{2d} \to S^{(1)} \times S^{(2)}$ and $\tilde{f} := (f \circ \Psi) J_\Psi$. Then $\tilde{f} \in G^\delta([0,1]^{2d})$.

Proof. Lemma 4.8 with $N = \{\}$. □

Lemma 4.10. *Suppose $1 \le p \le q$ are integers, B is a bounded subset of a $(p-1)$-dimensional hyperplane not containing 0, so that $P(B) \subset \mathbb{R}^p$, and $\Omega \subset \mathbb{R}^{q-p}$. Define $N := \{1, \dots, p\}$ and suppose $f(t) \in G_N^{\delta,\alpha}(P(B) \times \Omega)$,* i.e. $\exists\, A_0, A_1 > 0$ *independent of $\nu \in \mathbb{N}_0^q$, and $t \in (P(B)\backslash\{0\}) \times \Omega$ such that*

$$|D^\nu f(t)| \le A_0 A_1^{|\nu|} (\nu!)^\delta \|t_N\|^{\min(\alpha-\nu_N,0)}. \tag{4.32}$$

Consider a nonlinear mapping $\Lambda : [0,1] \times B \times \Omega \to P(B) \times \Omega$,

$$(t_1, \dots, t_q) = \Lambda(\zeta) := (\zeta_1, \zeta_1\zeta_2, \dots, \zeta_1\zeta_p, \zeta_{p+1}, \dots, \zeta_q). \tag{4.33}$$

Then $J_\Lambda = \zeta_1^{p-1}$ and $\tilde f := (f \circ \Lambda)(\zeta)\zeta_1^{p-1} \in G_{\{1\}}^{\delta,\tilde\alpha}([0,1] \times B \times \Omega)$ with $\tilde\alpha = \alpha + p - 1$, i.e. $\exists\, C_0, C_1 > 0$ *independent of $\nu \in \mathbb{N}_0^q$, and $\zeta \in (0,1] \times B \times \Omega$ such that*

$$|D^\nu \tilde f(\zeta)| \le C_0 C_1^{|\nu|} (\nu!)^\delta |\zeta_1|^{\min(\alpha+p-1-\nu_1,0)}. \tag{4.34}$$

Proof. The chain rule gives for $t = \Lambda(\zeta)$

$$D_{\zeta_i}^{\nu_i}(f \circ \Lambda)(\zeta) = \begin{cases} (D_{t_1} + \zeta_2 D_{t_2} + \ldots + \zeta_p D_{t_p})^{\nu_1} f(t), & i = 1, \\ (\zeta_1 D_{t_i})^{\nu_i} f(t), & i = 2, \dots, p \\ D_{t_i}^{\nu_i} f(t), & i = p+1, \dots, q. \end{cases} \tag{4.35}$$

We abbreviate $\kappa_\nu := \nu_2 + \ldots + \nu_p$, then

$$D_\zeta^\nu (f \circ \Lambda)(\zeta) = D_{\zeta_1}^{\nu_1}\big(\zeta^{\kappa_\nu} D_{(t_2,\dots,t_q)}^{(\nu_2,\dots,\nu_q)} f(t)\big) = \sum_{i=0}^{\min(\nu_1,\kappa_\nu)} \binom{\nu_1}{i} D_{\zeta_1}^i(\zeta_1^{\kappa_\nu}) D_{\zeta_1}^{\nu_1 - i}\big(D_{(t_2,\dots,t_q)}^{(\nu_2,\dots,\nu_q)} f(t)\big). \tag{4.36}$$

The chain rule (4.35) and the multinomial theorem yield

$$D_{\zeta_1}^{\nu_1-i}\big(D_{(t_2,\dots,t_q)}^{(\nu_2,\dots,\nu_q)} f(t)\big) = \sum_{\substack{\mu \in \mathbb{N}_0^p, \\ |\mu| = \nu_1 - i}} \binom{\nu_1 - i}{\mu} \zeta_2^{\mu_2} \dots \zeta_p^{\mu_p} D_t^{\nu_{i,\mu}^*} f(t),$$
$$\nu_{i,\mu}^* = (\mu_1, \nu_2 + \mu_2, \dots, \nu_p + \mu_p, \nu_{p+1}, \dots, \nu_q). \tag{4.37}$$

By assumption $f \in G_N^{\delta,\alpha}(P(B) \times \Omega)$ yielding for $0 \le i \le \min(\nu_1, \kappa_\nu)$

$$\begin{aligned} \big|D_{\zeta_1}^i(\zeta_1^{\kappa_\nu}) D_t^{\nu_{i,\mu}^*}(f(t))\big| &\le \frac{\kappa_\nu!}{(\kappa_\nu - i)!} \zeta_1^{\kappa_\nu - i} A_0 A_1^{|\nu_{i,\mu}^*|} (\nu_{i,\mu}^*!)^\delta \|(t_1, \dots, t_p)\|^{\min(\alpha-\kappa_\nu-|\mu|,0)} \\ &\le \tilde A_0 \tilde A_1^{|\nu|} (\nu!)^\delta |\zeta_1|^{\min(\alpha-\nu_1,0)}, \end{aligned} \tag{4.38}$$

where the last inequality holds, since $|\mu| = \nu_1 - i$; $a + \min(b,0) \ge \min(a+b,0)$ if $a \ge 0$;

$$\frac{\kappa_\nu!}{(\kappa_\nu - i)!}(\nu_{i,\mu}^*!)^\delta \le \left(\frac{\kappa_\nu!}{(\kappa_\nu - i)!}|\nu_{i,\mu}^*|!\right)^\delta \le \left(\frac{\kappa_\nu!}{(\kappa_\nu - i)!} q^{|\nu_{i,\mu}^*|} \nu_1!(\kappa_\nu - i)!\nu_{p+1}! \dots \nu_q!\right)^\delta \le q^{2\delta|\nu|}(\nu!)^\delta$$

and

$$\zeta_1 \le \|\zeta_1(1, \zeta_2, \dots, \zeta_p)\| \le C(B,q) \cdot \zeta_1,$$

where the constant $C(B,q)>0$ is independent of ζ and ν. The estimate

$$\sum_{i=0}^{\min(\nu_1,\kappa_\nu)} \binom{\nu_1}{i} \sum_{\substack{\mu\in\mathbb{N}_0^p,\\ |\mu|=\nu_1-i}} \binom{\nu_1-i}{\mu} \zeta_2^{\mu_2}\dots\zeta_p^{\mu_p} \le \sum_{i=0}^{\nu_1}\binom{\nu_1}{i}(1+\zeta_2+\ldots+\zeta_p)^{\nu_1-i} = (2+\zeta_2+\ldots+\zeta_p)^{\nu_1}$$

together with (4.36), (4.37) and (4.38) yields

$$\left|D_\zeta^\nu(f\circ\Lambda)(\zeta)\right| \le C_0 C_1^{|\nu|}(\nu!)^\delta|\zeta_1|^{\min(\alpha-\nu_1,0)}. \tag{4.39}$$

With similar arguments we obtain the asserted estimate for $\tilde f(\zeta)=(f\circ\Lambda)(\zeta)\zeta_1^{p-1}$:

$$\begin{aligned}
|D_\zeta^\nu\tilde f(\zeta)| &= |D_{\zeta_1}^{\nu_1}\big(\zeta_1^{p-1}D_{(\zeta_2,\dots,\zeta_q)}^{(\nu_2,\dots,\nu_q)}(f\circ\Lambda)(\zeta)\big)|\\
&\le \sum_{i=0}^{\min(\nu_1,p-1)}\binom{\nu_1}{i}\left|D_{\zeta_1}^i(\zeta_1^{p-1})D_{(\zeta_1,\zeta_2,\dots,\zeta_q)}^{(\nu_1-i,\nu_2,\dots,\nu_q)}(f\circ\Lambda)(\zeta)\right|\\
&\le \sum_{i=0}^{\min(\nu_1,p-1)}\binom{\nu_1}{i}\frac{(p-1)!}{(p-1-i)!}\zeta_1^{p-1-i}C_0C_1^{|\nu|-i}((\nu_1-i)!\nu_2!\dots\nu_q!)^\delta|\zeta_1|^{\min(\alpha-\nu_1+i,0)}\\
&\le \tilde C_0\tilde C_1^{|\nu|}(\nu!)^\delta|\zeta_1|^{\min(\alpha+p-1-\nu_1,0)}.
\end{aligned} \tag{4.40}$$

This finishes the proof. □

Proof of Theorem 4.2. We recall the sequence of transformations from the previous section

$$\begin{aligned}
I=\int_{x\in S_d}\int_{y\in S_d}G(x,y)\,\mathrm{d}y\mathrm{d}x &\overset{\text{Steps 1, 2}}{=} \sum_{j=1}^m\sum_{N\subset M}\sum_{\sigma\in\{-,+\}}\int_{(\check x,\check y,\tilde z)\in D_j^{N,\sigma}}\int_{\tilde x\in E_{N,M\setminus N}^\sigma(\tilde z)} g_2(\tilde z,\tilde x,\check x,\check y)\,\mathrm{d}\tilde x\,\mathrm{d}\tilde z\,\mathrm{d}\check y\,\mathrm{d}\check x\\
&\overset{\text{Step 3}}{=} \sum_{j=1}^m\sum_{N\subset M}\sum_{\sigma\in\{-,+\}}\int_{(s,u)\in[0,1]\times B_j^{N,\sigma}}\int_{\tilde x\in[0,1]^k} g_3(s,u,\tilde x)\,\mathrm{d}\tilde x\,\mathrm{d}u\,\mathrm{d}s\\
&\overset{\text{Step 4}}{=} \int_{\zeta\in[0,1]^{2d}}\tilde g(\zeta)\,\mathrm{d}\zeta.
\end{aligned} \tag{4.41}$$

As asserted, the integrand G satisfies Assumption 4.1, hence a direct application of Lemma 4.7 yields

$$g_2(\tilde z,\tilde x,\check x,\check y)\in G^{\delta,\alpha}_{\{1,\dots,k,2k+1,\dots 2d\}}(\Omega),$$
$$\text{with}\quad \Omega=\bigcup_{j=1}^m\bigcup_{N\subset M}\bigcup_{\sigma\in\{-,+\}}\big\{(\tilde z,\tilde x,\check x,\check y)|(\check x,\check y,\tilde z)\in D_j^{N,\sigma},\ \tilde x\in E_{N,M\setminus N}^\sigma(\tilde z)\big\}. \tag{4.42}$$

Further, we transform the simplex $E_{N,M\setminus N}^\sigma$ to S_k by (3.29) and then to $[0,1]^k$ by introducing the simplex coordinates and denote the above transformation by $\psi(\tilde z,\tilde x,\check x,\check y)$. Clearly ψ is a polynomial with $J_\psi\neq 0$ and the assumptions of Lemma 4.8(*ii*) are satisfied with $q=q'=2d$, $\Psi=\psi$ and $f=g_2$, thus

$$\tilde g_2(\check x,\check y,\tilde z,\tilde x):=(g_2\circ\psi)(\tilde z,\tilde x,\check x,\check y)J_\psi\in G^{\delta,\alpha}_{\{1,\dots,2d-k\}}(\Omega),$$
$$\Omega=\bigcup_{j=1}^m\bigcup_{N\subset M}\bigcup_{\sigma\in\{-,+\}}\big\{(\check x,\check y,\tilde z,\tilde x)|(\check x,\check y,\tilde z)\in D_j^{N,\sigma},\ \tilde x\in[0,1]^k\big\}.$$

Recall that each $D_j^{N,\sigma} = P(B_j^{N,\sigma})$ is a pyramid. Hence the assumptions of Lemma 4.10 are satisfied with $p = 2d - k$, $q = 2d$ and $f = \tilde{g}_2$ yielding

$$g_3(s,u,\tilde{x}) \in G_{\{1\}}^{\delta,\alpha+2d-k-1}(\Omega), \quad \Omega = \bigcup_{j=1}^{m} \bigcup_{N\subset M} \bigcup_{\sigma\in\{-,+\}} \big\{(s,u,\tilde{x}) | s \in [0,1],\ u \in B_j^{N,\sigma},\ \tilde{x} \in [0,1]^k\big\}.$$

Note that $B_j^{N,\sigma}$ is a tensor product of simplices. We parameterize each of these simplices by the simplex coordinates and obtain

$$\tilde{g}(\zeta) \in G_{\{1\}}^{\delta,\alpha+2d-k-1}([0,1]^{2d}),$$

which follows directly from Lemma 4.8. □

4.4. **Technical results**

Finally we prove two technical lemmas. Lemma 4.11 is required in the proof of Lemmas 4.7 and 4.11 is used in the proof of Lemma 4.12.

Lemma 4.11. *For arbitrary $x, y \in [0,1]^2$ there holds*

$$\|(x_1(1-x_2), x_2)\| \sim \|(x_1, x_2)\|, \tag{4.43}$$

$$\|(x_1(1-x_2) - y_1(1-y_2), x_2, y_2)\| \sim \|(x_1 - y_1, x_2, y_2)\|. \tag{4.44}$$

Proof. We prove the lemma for $\|\cdot\|_1$. Considering (4.43) we note that $\|(x_1,x_2)\|_1 \le 2$. Then

$$\|(x_1,x_2)\|_1 \ge \|(x_1(1-x_2),x_2)\|_1 \ge \left\{ \begin{array}{ll} \frac{1}{2}, & x_1 \ge \frac{1}{2} \\ \frac{1}{2}\|(x_1,x_2)\|_1, & x_1 < \frac{1}{2} \end{array} \right\} \ge \frac{1}{4}\|(x_1,x_2)\|_1 \tag{4.45}$$

and (4.43) follows. We prove (4.44) in several steps. On the one hand there holds

$$f := x_1(1-x_2) - y_1(1-y_2) \equiv (x_1-y_1)(1-x_2) - y_1(x_2-y_2), \tag{4.46}$$

thus using the triangle inequality we have

$$\|(f,x_2,y_2)\|_1 \le |x_1-y_1| + 2x_2 + 2y_2 \le 2\|(x_1-y_1,x_2,y_2)\|_1. \tag{4.47}$$

On the order to show the reverse estimate we define $z := |x_1 - y_1|$, yielding

$$|f| = |z(1-x_2) - y_1 \mathrm{sign}\{x_1-y_1\}(x_2-y_2)| \tag{4.48}$$

and consider the three following cases.

Consider the case $(x_1-y_1)(x_2-y_2) < 0$. Then

$$z(1-x_2) - y_1\mathrm{sign}\{x_1-y_1\}(x_2-y_2) \ge z(1-x_2) \ge 0 \tag{4.49}$$

and thus using (4.45)

$$\|(f,x_2,y_2)\|_1 \ge z(1-x_2) + x_2 + y_2 \ge \frac{1}{4}\|(z,x_2,y_2)\|_1. \tag{4.50}$$

Consider the case $(x_1-y_1)(x_2-y_2) > 0$ and either $z \le x_2$ or $z \le y_2$. Then

$$\|(f,x_2,y_2)\|_1 \ge \|(0,x_2,y_2)\|_1 \ge \frac{1}{2}\|(z,x_2,y_2)\|_1. \tag{4.51}$$

Consider the case $(x_1 - y_1)(x_2 - y_2) > 0$ and $z > \max\{x_2, y_2\}$. Let us show that

$$|f| \geq z - \max\{x_2, y_2\}. \tag{4.52}$$

Indeed, if $x_2 \geq y_2$, then

$$x_1 \geq y_1, \qquad z = x_1 - y_1 \geq 0, \qquad (x_1 - y_1) - x_1x_2 = z - x_1x_2 \geq z - x_2 > 0, \tag{4.53}$$

which yields

$$|f| = |x_1 - y_1 - x_1x_2 + y_1y_2| = x_1 - y_1 - x_1x_2 + y_1y_2 \geq z - x_2. \tag{4.54}$$

Further, for $x_2 \leq y_2$ we have

$$x_1 \leq y_1, \qquad z = y_1 - x_1 \geq 0, \qquad (y_1 - x_1) - y_1y_2 = z - y_1y_2 \geq z - y_2 > 0, \tag{4.55}$$

which gives

$$|f| = |x_1 - y_1 - x_1x_2 + y_1y_2| = y_1 - x_1 + x_1x_2 - y_1y_2 \geq y_1 - x_1 - y_1y_2 \geq z - y_2 \tag{4.56}$$

and (4.52) holds true. Define $v := \min\{x_2, y_2\}$, $w := \max\{x_2, y_2\}$, then $z > w$ and

$$\|(f, x_2, y_2)\|_1 \geq \|(z - \max\{x_2, y_2\}, x_2, y_2)\|_1 = \|(z - w, v, w)\|_1 = z + v \geq \frac{1}{2}\|(z, v, w)\|_1 \geq \frac{1}{2}\|(z, x_2, y_2)\|_1. \tag{4.57}$$

The proof is complete. □

Lemma 4.12. *Define* $\sigma_{\check{x}} := 1 - \|\check{x}\|_1$. *Then*

$$(\tilde{x}, \check{x}) \in S_k \times S_{d-k} \iff (\sigma_{\check{x}}\tilde{x}, \check{x}) \in S_d, \tag{4.58}$$

$$\|(\tilde{x} - \tilde{y}, \check{x}, \check{y})\| \sim \|(\sigma_{\check{x}}\tilde{x} - \sigma_{\check{y}}\tilde{y}, \check{x}, \check{y})\|. \tag{4.59}$$

Proof. Equivalence (4.58) follows directly from the definition of S_d. Define $u := \|\check{x}\|_1$, $v := \|\check{y}\|_1$. Note that $u, v \in [0, 1]$ and

$$\|(\sigma_{\check{x}}\tilde{x} - \sigma_{\check{y}}\tilde{y}, \check{x}, \check{y})\|_1 = \|((1 - u)\tilde{x} - (1 - v)\tilde{y}, u, v)\|_1. \tag{4.60}$$

Thus by Lemma 4.11 we obtain

$$\frac{1}{4k}\|(\tilde{x} - \tilde{y}, \check{x}, \check{y})\|_1 = \frac{1}{4k}\|(\tilde{x} - \tilde{y}, u, v)\|_1 \leq \|((1 - u)\tilde{x} - (1 - v)\tilde{y}, u, v)\|_1 \leq 2k\|(\tilde{x} - \tilde{y}, u, v)\|_1 = 2k\|(\tilde{x} - \tilde{y}, \check{x}, \check{y})\|_1. \tag{4.61}$$

□

5. Singular integrals over parallelotopes in $\mathbb{R}^d$

5.1. Introduction

We want to compute the integral over two d-dimensional parallelotopes (images of d-dimensional cubes under affine transformations)

$$I = \int_{x \in P^{(1)}} \int_{y \in P^{(2)}} g(x, y) \, \mathrm{d}y \, \mathrm{d}x$$

where we make the following assumptions:

Assumption 5.1. *$P^{(1)}, P^{(2)} \subset \mathbb{R}^d$ are d-dimensional closed parallelotopes with positive volume. Moreover, $P^{(1)} \cap P^{(2)}$ is either empty, or a k-dimensional parallelotope side with $k \in \{0, \ldots, d\}$.*

This assumption is satisfied if $P^{(j)}$ are parallelotopes in a regular finite element mesh.

Assumption 5.2. *The function $g(x,y)$ can be written as $g(x,y) = F(x,y,y-x)$ with $F \in G^{\delta,\alpha}_{\{2d+1,\dots,3d\}}(P^{(1)} \times P^{(2)} \times (P^{(2)} - P^{(1)}))$ where $\delta \geq 1$, $\alpha \in \mathbb{R}$. If $P^{(1)} \cap P^{(2)}$ is nonempty we assume $\alpha > k - 2d$, this implies $g \in L^1(P^{(1)} \times P^{(2)})$.*

Let $J := [0,1]$. Then we can use a change of variables from $x \in P^{(1)}$, $y \in P^{(2)}$ to $u, v \in J^d$ with $x = v^{(1,0)} + A^{(1)}u$, $y = v^{(2,0)} + A^{(2)}v$ and obtain

$$I = \int_{u \in J^d} \int_{v \in J^d} G(u,v) \mathrm{d}v \, \mathrm{d}u \tag{5.1}$$

with $G(u,v)$ given by (3.4).

If the intersection $P^{(1)} \cap P^{(2)}$ is empty (*i.e.*, the parallelotopes have a positive distance) we obtain as in Proposition 3.3 that $G \in G^{\delta}(J^{2d})$ and $|I - Q_n \otimes \cdots \otimes Q_n(G)| \leq C \exp(-rn^{1/\delta})$.

If the intersection $P^{(1)} \cap P^{(2)}$ is a k-dimensional parallelotope side with $k \in \{0,\dots,d\}$, then we can choose $v^{(j,0)}$ and $A^{(j)}$ such that $v^{(1,0)} = v^{(2,0)}$ and the first k columns of $A^{(1)}, A^{(2)}$ coincide. Therefore we obtain as in Section 3.1 that we can write G in the form

$$\begin{aligned} &G(u,v) = H(u,v,\hat{v}-\hat{u},\check{u},\check{v}) \\ &H(u,v,\xi,\eta,\zeta) \in G^{\delta,\alpha}_{\{2d+1,\dots,4d-k\}}\left(J^d \times J^d \times [-1,1]^k \times J^{d-k} \times J^{d-k}\right). \end{aligned} \tag{5.2}$$

5.2. Transformations for cubes

(1) Let us first assume $k \geq 1$. We now use $\hat{z} := \hat{y} - \hat{x}$ to transform $(\hat{x},\hat{y}) \in J^k \times J^k$ to $(\hat{z},\hat{x})$ with $\hat{z} \in J^k - J^k = [-1,1]^k$, $\hat{x} \in F_k(\hat{z}) := J^k \cap (J^k - z)$ so that for $g_1(\hat{x},\hat{y},\check{x},\check{y}) := G(\hat{x},\hat{y},\check{x},\check{y})$ we have

$$I = \int_{\hat{z} \in [-1,1]^k} \int_{\hat{x} \in F_k(\hat{z})} \int_{\check{x} \in J^{d-k}} \int_{\check{y} \in J^{d-k}} g_1(\hat{x},\hat{x}+\hat{z},\check{x},\check{y}) \, \mathrm{d}\check{y} \, \mathrm{d}\check{x} \, \mathrm{d}\hat{x} \, \mathrm{d}\hat{z}. \tag{5.3}$$

We now split $[-1,1]^k$ along the octants into 2^k cubes: with $M = \{1,\dots,k\}$ we have with $C_{N^-,N^+} = \{z \mid z_{N^-} \in [-1,0]^{\#N^-},\ z_{N^+} \in [0,1]^{\#N^+}\}$

$$[-1,1]^k = \bigcup_{N \subset M} C_{N,M\setminus N}$$

$$\hat{z} \in C_{N^-,N^+} \quad \Longrightarrow \quad F_k(\hat{z}) = -\hat{z}^{(N^-)} + [0, 1-|\hat{z}_1|] \times \ldots \times [0, 1-|\hat{z}_k|] =: F_{N^-,N^+}(\hat{z}) \tag{5.4}$$

and get

$$I = \sum_{N \subset M} \int_{\hat{z} \in C_{N,M\setminus N}} \int_{\hat{x} \in F_{N,M\setminus N}(\hat{z})} \int_{\check{x} \in J^{d-k}} \int_{\check{y} \in J^{d-k}} g_1(\hat{x},\hat{x}+\hat{z},\check{x},\check{y}) \, \mathrm{d}\check{y} \, \mathrm{d}\check{x} \, \mathrm{d}\hat{x} \, \mathrm{d}\hat{z} \tag{5.5}$$

which is a sum over 2^k terms. Note that $g_2(\hat{z},\hat{x},\check{x},\check{y}) := g_1(\hat{x},\hat{x}+\hat{z},\check{x},\check{y})$ is Gevrey unless $\|(\hat{z},\check{x},\check{y})\| = 0$.

(2) We now note that $w := (\hat{z},\check{x},\check{y}) \in C_{N,M\setminus N} \times J^{d-k} \times J^{d-k} =: D^N \subset \mathbb{R}^{\tilde{d}}$ with $\tilde{d} = k + 2(d-k) = 2d-k$. Then D^N is a Cartesian product of $m = 2d-k$ pyramids (since $[0,1]$ is a pyramid with base $B = \{1\}$). By Proposition 3.5 we can split D^N into $m = 2d-k$ pyramids, yielding $D^N = D^N_1 \cup \cdots \cup D^N_m$.

(3) We use the parameterizations (3.20) to transform each D^N_j to $[0,1]^{2d-k}$. Note that the parameter $s \in [0,1]$ satisfies $s \sim \|w\|$, and that the determinant of the Jacobian gives a factor of $s^{\tilde{d}-1} = s^{2d-k-1}$. We will finally obtain with $\zeta_1 = s$

$$I = \int_{\zeta \in [0,1]^{2d}} \tilde{g}(\zeta) \mathrm{d}\zeta, \qquad \tilde{g}(\zeta) := \sum_{N \subset M} \sum_{j=1}^{m} \tilde{g}_{N,j}(\zeta) \mathrm{d}\zeta \tag{5.6}$$

where $\tilde{g}_{N,j} \in G^{\delta,\tilde{\alpha}}_{\{1\}}(J^{2d})$.

TABLE 2. Number K of integrals after transformation in (5.7).

d	$k=0$	$k=1$	$k=2$	$k=3$	$k=4$
1	2	2			
2	4	6	8		
3	6	10	16	24	
4	8	14	24	40	64

So far we assumed $k \geq 1$ so that we need to deal with the variables $\hat{x}, \hat{y}$ in the intersection cube. In the case $k = 0$ where the two original parallelotopes touch at a vertex there are no variables $\hat{x}, \hat{y}$ and we obtain instead of (5.3)

$$I = \int_{\check{x} \in J^d} \int_{\check{y} \in J^d} g_1(\check{x}, \check{y}) \mathrm{d}\check{y} \, \mathrm{d}\check{x}.$$

Therefore we can skip step (1). In step (2) we split the domain $D = J^d \times J^d$ into $m = 2d$ pyramids.

Therefore the total number K of terms we obtain is always

$$K = 2^k(2d - k). \tag{5.7}$$

Table 2 shows K for $d = 1, \ldots, 4$.

Note that in the case $d = 1$ both simplices and parallelotopes are just intervals, and we obtain the same transformations.

5.3. Quadrature and error estimate

We defined the transformed integrand $\tilde{g}$ in (5.6). The main result of this section is the following theorem.

Theorem 5.3. *Let $k \in \{0, \ldots, d\}$, $\delta \geq 1$, $\alpha > k - 2d$. Suppose G satisfies (5.2) and $\tilde{g}_{N,j}$ are obtained from G by the sequence of the coordinate transformations given by Steps 1–2 from the previous section. Then*

$$\tilde{g}(\zeta) \in G^{\delta,\tilde{\alpha}}_{\{1\}}(J^{2d}), \qquad \textit{with} \qquad \tilde{\alpha} = \alpha + 2d - k - 1,$$

i.e. $\exists\, C_0, C_1 > 0$ independent of $\nu \in \mathbb{N}_0^{2d}$ and $\zeta \in (0,1] \times [0,1]^{2d-1}$ such that

$$|D^\nu_\zeta \tilde{g}(\zeta)| \leq C_0 C_1^{|\nu|} (\nu!)^\delta |\zeta_1|^{\min(\tilde{\alpha} - \nu_1, 0)}, \quad \tilde{\alpha} = \alpha + 2d - k - 1.$$

Definition 5.4. Let $\tilde{Q}^{k,d}_{n,m}$ be the quadrature rule on J^{2d} such that

$$\tilde{Q}^{k,d}_{n,m} G := [Q_{n,m} \otimes \underbrace{Q_n \cdots \otimes Q_n}_{2d-1 \text{ times}}] \tilde{g},$$

where $Q_{n,m}$ is the quadrature rule in Definition 2.4 and $\tilde{g}$ is given by (5.6).

The exponential convergence of the quadrature rule $\tilde{Q}^{k,d}_{n,m}$ is a corollary of Theorem 5.3 and Proposition 2.8:

Theorem 5.5. *Let $k \in \{0, \ldots, d\}$, $\delta \geq 1$, $\alpha > k - 2d$. Suppose G satisfies (5.2). Let $b > 0$ and $m = \lceil bn^{1/\delta} \rceil$. Then there exist $r, r', C > 0$ so that for all $n \in \mathbb{N}$*

$$\left| \int_{x \in J^d} \int_{y \in J^d} G(x,y) \, \mathrm{d}y \mathrm{d}x - \tilde{Q}^{k,d}_{n,m} G \right| \leq C \exp(-rn^{1/\delta}) \leq C \exp(-r' N^{1/(2d\delta+1)}),$$

where $N = O(n^{2d+1/\delta})$ is the number of function evaluations in the quadrature rule $\tilde{Q}^{k,d}_{n,m}$.

The proof of Theorem 5.3 is similar to the proof of Theorem 4.2 and requires the following auxiliary lemma.

Lemma 5.6. *Let $g_2(\hat{z},\hat{x},\check{x},\check{y}) = G(\hat{x},\hat{x}+\hat{z},\check{x},\check{y})$ and (5.2) holds true. Then*

$$g_2(\hat{z},\hat{x},\check{x},\check{y}) \in G^{\delta,\alpha}_{\{1,\dots,k,2k+1,\dots,2d\}}(\Omega'), \quad \Omega' = \big\{(\hat{z},\hat{x})|\hat{z}\in[-1,1]^k,\ \hat{x}\in F_k(\hat{z})\big\}\times J^{d-k}\times J^{d-k},$$

i.e. $\exists\, C_0, C_1 > 0$ independent of $\nu^\circ \in \mathbb{N}_0^k$, $\nu^* \in \mathbb{N}_0^{2d-k}$ and $(\hat{z},\hat{x},\check{x},\check{y}) \in \Omega$ such that

$$|D^{\nu^\circ}_{\hat{x}} D^{\nu^*}_{(\hat{z},\check{x},\check{y})} g_2(\hat{z},\hat{x},\check{x},\check{y})| \le C_0 C_1^{|\nu^\circ|+|\nu^*|}(\nu^\circ!\nu^*!)^\delta \|(\hat{z},\check{x},\check{y})\|^{\min(\alpha-|\nu^*|,0)}.$$

Proof. The proof follows directly from Lemma 4.8. Indeed, with $\phi(\hat{z},\hat{x},\check{x},\check{y}) := (\hat{x},\check{x},\hat{x}+\hat{z},\check{y},\hat{z},\check{x},\check{y})$ we have

$$g_2(s) = (H\circ\phi)(s), \quad s := (\hat{z},\hat{x},\check{x},\check{y}).$$

Then the assumptions of Lemma 4.8 are satisfied with $f = H$, $\Psi = \phi$,

$$\Omega := J^d\times J^d\times[-1,1]^k\times J^d\times J^d, \quad \Omega' = \big\{(\hat{z},\hat{x})|\hat{z}\in[-1,1]^k,\ \hat{x}\in F_k(\hat{z})\big\}\times J^{d-k}\times J^{d-k}$$

and N such that $t_N = s_N = (\hat{z},\check{x},\check{y})$ up to reordering of variables. □

Proof of Theorem 5.3. We recall the sequence of transformations

$$\begin{aligned} I = \int_{x\in J^d}\int_{y\in J^d} G(x,y)\,\mathrm{d}y\,\mathrm{d}x &\overset{\text{Steps 1, 2}}{=} \sum_{N\subset M}\sum_{j=1}^m \int_{(\hat{z},\check{x},\check{y})\in D_j^N}\int_{\hat{x}\in F_{N,M\setminus N}(\hat{z})} g_2(\hat{z},\hat{x},\check{x},\check{y})\,\mathrm{d}\check{y}\,\mathrm{d}\check{x}\,\mathrm{d}\hat{x}\,\mathrm{d}\hat{z} \\ &\overset{\text{Step 3}}{=} \sum_{N\subset M}\sum_{j=1}^m \int_{\zeta\in[0,1]^{2d}} \hat{g}_{N,j}(\zeta)\,\mathrm{d}\zeta. \end{aligned}$$

Lemma 5.6 yields directly

$$g_2(\hat{z},\hat{x},\check{x},\check{y}) \in G^{\delta,\alpha}_{\{1,\dots,k,2k+1,\dots,2d\}}(\Omega), \qquad \Omega := \{\hat{z}\in[-1,1]^k,\ \hat{x}\in F_k(\hat{z})\}\times J^{d-k}\times J^{d-k}.$$

Further we transform $\psi : F_{N,M\setminus N} \to J^k$ by using parameterizations (5.4). The transformation ψ is a polynomial and $J_\psi \neq 0$. Thus, assumptions of Lemma 4.8(*ii*) are satisfied with $q = q' = 2d$, $\Psi = \psi$ and $f = g_2$, hence

$$\tilde{g}_2(\check{x},\check{y},\tilde{z},\tilde{x}) := (g_2\circ\psi)(\tilde{z},\tilde{x},\check{x},\check{y})J_\psi \in G^{\delta,\alpha}_{\{1,\dots,2d-k\}}(\Omega), \quad \Omega = \bigcup_{j=1}^m\bigcup_{N\subset M}\big\{(\check{x},\check{y},\tilde{z},\tilde{x})|(\check{x},\check{y},\tilde{z})\in D_j^N,\ \tilde{x}\in[0,1]^k\big\}.$$

Furthermore, each D_j^N is a pyramid and might be written in the form $P(J^{2d-k-1})$. Hence the assumptions of Lemma 4.10 are satisfied for every summand with $p = 2d-k$, $B = J^{2d-k-1}$ and $\Omega = [0,1]^k$, hence by Lemma 4.8 $g_{N,j}(\zeta) \in G^{\delta,\hat{\alpha}}_{\{1\}}(J^{2d})$. □

6. Numerical examples

6.1. Gevrey functions on an interval

In the case of $g \in G^\delta([a,b])$ with $\delta = 1$ the function g is analytic in a neighborhood of $[a,b]$, and the exponential convergence $|\mathcal{I}g - Q_N g| \le C\exp(-rN)$ of Gaussian quadrature is known to be sharp.

The case $g \in G^{\delta,\alpha}([0,1])$ with $\delta = 1$, $\alpha > -1$ corresponds to a function g which is analytic on $(0,1]$, but may have an algebraic singularity at 0. The method of composite Gauss quadrature with geometric subdivision was first used in [20] and yields $|\mathcal{I}g - Q_{n,m}g| \le C\exp(-rN^{1/2})$ where $m = \lceil bn\rceil$ with b as in Theorem 2.5

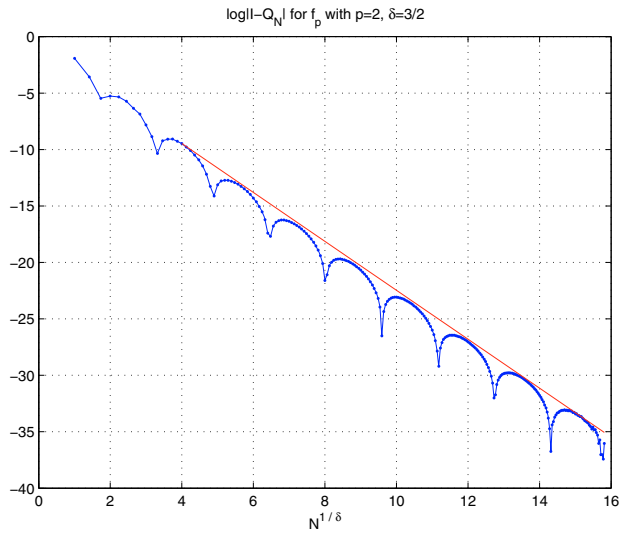

FIGURE 3. $\log|\mathcal{I}f_p - Q_N f_p|$ for function f_p in (6.1) with $p = 2$, $\delta = \frac{3}{2}$ and $N = 1, \ldots, 250$. The horizontal axis is $N^{1/\delta}$, the line corresponds to $|\mathcal{I}f_p - Q_N f_p| = C\exp(-rN^{1/\delta})$.

and $N = O(n^2)$ denotes the total number of quadrature points. Note that the sinc method of Stenger [22] also yields the convergence rate $C\exp(-rN^{1/2})$. It is shown in [22] that this rate is optimal among all sequences of quadrature formulas for a certain class of analytic functions on an interval with endpoint singularities.

In the case of a Gevrey function $g \in G^\delta([a,b])$ with $\delta > 1$ we obtain the rate $|\mathcal{I}g - Q_N g| \le C\exp(-rN^{1/\delta})$. We want to provide numerical evidence that this rate is sharp: We consider the function

$$f_p(x) := \begin{cases} \exp(x^{-p}) & \text{for } x > 0 \\ 0 & \text{for } x \le 0 \end{cases} \tag{6.1}$$

with $p > 0$ on the interval $[-1, 1]$. Then we have

$$f_p \in G^\delta([-1,1]) \iff \delta \ge 1 + 1/p \tag{6.2}$$

see *e.g.* [2], p. 16. In Figure 3 we show $N^{1/\delta}$ on the horizontal axis, and $\log|\mathcal{I}f_p - Q_N f_p|$ on the vertical axis.

6.2. Integrals over simplices in $\mathbb{R}^2$ and $\mathbb{R}^3$

Here we consider for $d = 2, 3$ the integral (3.5) with $S^{(1)} = S_d$ and $S^{(2)} = ((y_1, \ldots, y_k, -y_{k+1}, \ldots, -y_d) \,|\, y \in S_d)$ where $k = 0, \ldots, d$, *i.e.*, the intersection $S^{(1)} \cap S^{(2)} = \{(\hat{x}, 0, \ldots, 0) \mid \hat{x} \in S_k\}$ is k-dimensional. Hence Assumption 3.1 is satisfied.

We use the integrand

$$g(x,y) = \|y - x\|^\alpha, \qquad \alpha = k - 2d + \beta \tag{6.3}$$

with $\beta > 0$, *i.e.*, the exponent is by β larger than the critical exponent $k-2d$ where $g \notin L^1(S^{(1)} \times S^{(2)})$. Therefore $g(x,y) = F(x,y,y-x)$ with $F(x,y,z) = \|z\|^\alpha$ and $F \in G^{\delta,\alpha}(S^{(1)} \times S^{(2)} \times (S^{(2)} - S^{(1)}))$ with $\delta = 1$. Hence Assumption 3.2 is satisfied. With $\hat{x} = (x_1, \ldots, x_k)$ and $\check{x} = (x_{k+1}, \ldots, x_d)$ we have $G(x,y) = \|(\hat{y} - \hat{x}, \check{x} + \check{y})\|^\alpha$ and $H(x,y,\hat{z},\check{x},\check{y}) = \|(\hat{z}, \check{x} + \check{y})\|^\alpha$.

In our numerical experiments we chose for each d and k the exponent α so that $\beta = 1/\pi$. We chose singularities very close to the nonintegrable case for *all* $k = 0, \ldots, d$ as a tough test for our algorithm. In applications

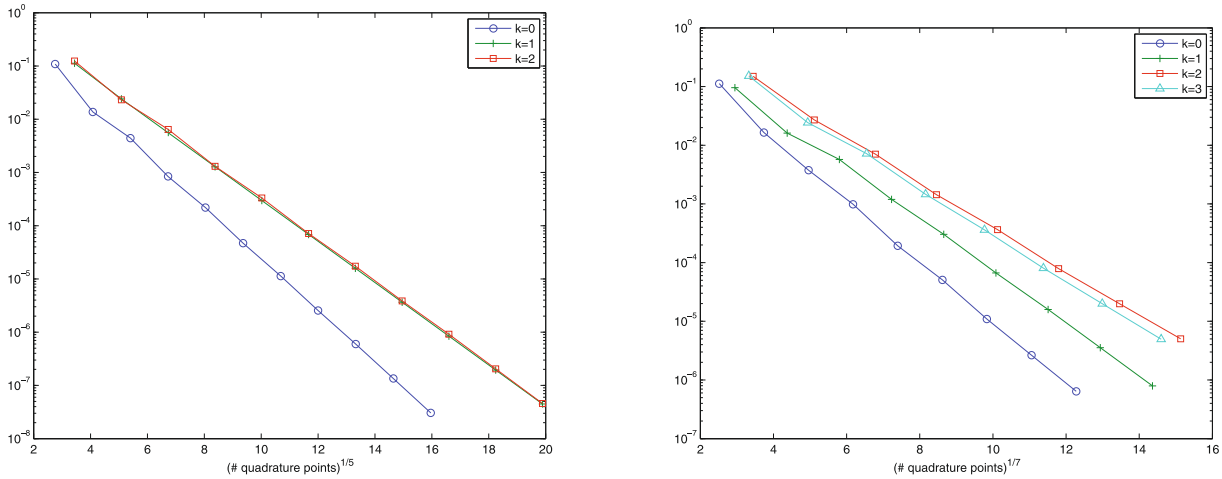

FIGURE 4. Relative errors $|\mathcal{Q}_N - I|/I$ for $d = 2$ (left) and $d = 3$ (right), with $k = 0, \ldots, d$.

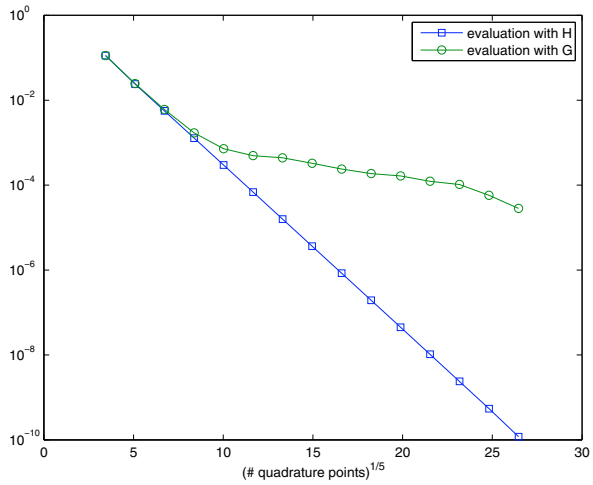

FIGURE 5. Relative error $|\mathcal{Q}_N - I|/I$ for naive evaluation of integrand G and improved algorithm evaluating H.

for integral equations one has a fixed integrand $g(x, y) \sim \|x - y\|^{\alpha_*}$ with $\alpha_* > -d$ for all k, and one would have $\beta_k := \alpha_* - (k - 2d) > d - k$.

We use Gaussian quadrature with n nodes for each of the smooth variables $\zeta_2, \ldots, \zeta_{2d}$. For the singular variable ζ_1 we 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 points on the subintervals. We use $n = 2, \ldots, 12$ for $d = 2$ and $n = 2, \ldots, 10$ for $d = 3$.

In Figure 4 we show on the vertical axis the relative error $|\mathcal{Q}_N - I|/I$ with a logarithmic scale, and on the horizontal axis $N^{1/(2d+1)}$ where

$$N = K \cdot \frac{1}{2}\tilde{n}(\tilde{n} + 1) \cdot n^{2d-1}$$

is the total number of quadrature points. The bound in Theorem 4.5 then corresponds to a straight line.

In implementation, particular attention must be paid to the numerical evaluation of the integrand as discussed in Section 3.4, Remark 3.7. To illustrate Remark 3.7 numerically, we show results for $d = 2$ and $k = 1$ in Figure 5: if we evaluate the function $G(x, y)$ using (3.39) and (3.38) we encounter dramatic subtractive cancellation.

If we use equations (3.55) and (3.54) to evaluate the function H the roundoff error does not affect the convergence behavior. We conclude with remarking that the instability due to subtractive cancellation which is apparent in Figure 5 is less pronounced for larger values of α in the integrand $g(x, y)$ in (6.3).

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