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Corrected trapezoidal rules for a class of singular functions

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A set of accurate quadrature rules applicable to a class of integrable functions with isolated singularities is designed and analysed theoretically in one and two dimensions. These quadrature rules are based on the trapezoidal rule with corrected quadrature weights for points in the vicinity of the singularity. To compute the correction weights, small-size ill-conditioned systems have to be solved. The convergence of the correction weights is accelerated by the use of compactly supported functions that annihilate boundary errors. Convergence proofs with error estimates for the resulting quadrature rules are given in both one and two dimensions. The tabulated weights are specific for the singularities under consideration, but the methodology extends to a large class of functions with integrable isolated singularities. Furthermore, in one dimension we have obtained a closed form expression based on which the modified weights can be computed directly.

Keywords: singular functions; quadrature methods; high order.

1. Introduction

This paper focuses on the design of accurate quadrature rules for functions with isolated singularities. The need to numerically evaluate such integrals arises in, e.g., methods based on boundary integral equations, where the fundamental solution, or Green's function, has an integrable singularity.

In the literature one can find several different approaches to the numerical integration of singular functions. These include different semianalytical techniques and singularity subtraction approaches (see Pozrikidis, 1992). Different mappings and changes of coordinates in order to remove the singularity have also been applied (see Duffy, 1982; Bruno & Kunyansky, 2001; Atkinson, 2004; Khayat & Wilton, 2005; Sidi, 2005; Mousavi & Sukumar, 2010). The approach that we will follow here is to modify the trapezoidal rule to render it high-order accurate for singular functions. The resulting quadrature rules are very attractive due to their simplicity—the trapezoidal rule is modified with a small number of correction weights, and the simple structure is retained.

The trapezoidal rule is spectrally accurate for smooth, compactly supported or periodic functions. For other functions it is in general at most second-order accurate. There are two sources of these larger errors: singularities and boundaries. Both of these error sources can be reduced by modifying the quadrature weights locally, in the vicinity of the singularity (which is assumed here to be isolated) or at the boundaries. Hence, by adjusting the weights locally, high-order-accurate versions of the trapezoidal rule can be constructed also in the presence of singularities and boundaries. The new weights are precomputed and tabulated; once constructed, the modified trapezoidal rule can easily be applied. In the case of a singularity, the modified weights are, however, specific to the singularity that is being considered.

The first singularity-corrected trapezoidal methods introduced in Rokhlin (1990) were restricted in practice to rather low orders of accuracy since the magnitude of the correction weights became very large for higher-order methods. To alleviate this problem, Alpert (1995) used more correction weights than the optimal number, and minimized their sum of squares. The integration interval is split at the singularity into two subintervals such that the singularity is always at a boundary. Kapur & Rokhlin (1997) introduced additional quadrature points and weights outside the interval of integration and could thereby obtain much smaller correction weights. Such a method is not always convenient to apply, and yet another approach by Alpert (1999), was to introduce a hybrid Gauss–trapezoidal rule, where a few of the regularly spaced nodes towards the interval end points are replaced with irregularly spaced nodes. The computed weights at the irregular nodes are both bounded and positive.

In the papers Rokhlin (1990), Alpert (1995, 1999) and Kapur & Rokhlin (1997), quadrature rules are designed for singular functions of the form $f(x) = \phi(x)s(x) + \psi(x)$ and $f(x) = \phi(x)s(x)$, where $\phi(x)$ and $\psi(x)$ are regular functions and $s(x)$ has an isolated integrable singularity such as $s(x) = |x|^\gamma$, $\gamma > -1$ or $s(x) = \log(|x|)$. The integration interval is split at the singularity, and for each subinterval there is a regular end and a singular end. Corrections to the trapezoidal rule are applied at both ends in order to reduce the boundary errors at the regular end and to control the error from the singularity and the boundary at the other end. Theoretical analysis is offered for all these methods.

It is inconvenient to split the domain of integration at the singularity in higher dimensions. Aguilar and Chen designed singularity-corrected trapezoidal rules for the $s(\mathbf{x}) = \log(|\mathbf{x}|)$ singularity in $\mathbb{R}^2$ (see Aguilar & Chen, 2002), and for $s(\mathbf{x}) = 1/|\mathbf{x}|$ in $\mathbb{R}^3$ (see Aguilar & Chen, 2005). The singularities are interior to the domain and a singularity correction in the interior is combined with boundary corrections to yield higher-order methods. No theoretical analysis is provided in these papers, but the expected order of accuracy is given for the method, which is consistent with numerical examples.

One procedure for constructing a set of increasingly accurate quadrature rules is to require the exact integration of monomials of increasing degree (see Keast & Lyness, 1979). A similar procedure is followed here to determine the modified weights of the corrected trapezoidal rules. The exact integration of monomials, up to a desired degree, multiplying the singular function $s(x)$ is first enforced for a specific uniform grid spacing h. This leads to a linear system of equations for the modified weights. The obtained correction weights will then depend on h. This is not very practical. Instead, one wants to use the converged weights that are defined as the weights obtained in the limit as $h \to 0$. They are grid independent, universal for the given singularity and can be tabulated once computed. As Aguilar & Chen (2002, 2005) note, the system to be solved for the weights becomes severely ill conditioned, more so for smaller h and multiprecision arithmetic is needed to perform this task.

Duan & Rokhlin (2009) apply similar techniques to design singularity-corrected trapezoidal rules for $s(\mathbf{x}) = \log(|\mathbf{x}|)$ singularities in two dimensions. However, they do not seek converged correction weights, but compute weights that depend on the grid size h. They are able to derive analytical, although very lengthy, expressions for the weights and thereby avoid solving an ill-conditioned system. The analytical formulas that they derive are, however, approximated numerically, but to very high accuracy. A theoretical proof is offered regarding the accuracy of the quadrature rules, using also some theoretical results developed in Lyness (1976).

In this paper we consider singularities of the kind $s(x) = |x|^\gamma$, $\gamma > -1$ in one dimension and $s(\mathbf{x}) = 1/|\mathbf{x}|$ in two dimensions. The singularities are interior to the domain. As in Aguilar & Chen (2002), our singularity corrections can be combined with boundary corrections (see Alpert, 1995) to reduce boundary errors as needed.

One difference in our approach compared with all previous works cited above lies in the procedure for computing the weights. The corrected trapezoidal rule is based on the punctured trapezoidal rule (excluding the point of singularity) together with a correction operator which is applied at grid points in the vicinity of the singularity. In order to accelerate the convergence of the weights, the boundary errors in the punctured trapezoidal rule must be reduced. The approach used previously is to introduce a boundary correction for the trapezoidal rule. Here, we suggest an alternative approach where we multiply $s(x)$ by a fixed, compactly supported function $g(x)$. This completely annihilates the boundary errors. The convergence rate of the weights will now instead depend on the number of derivatives of g that vanish at the point of singularity. This is proved for the one-dimensional case in Section 3; see Lemma 3.8. For the two-dimensional case, we cannot offer a rigorous proof, but note the same behaviour in practice. With a faster convergence rate for the weights, larger values of h can be used, which to some extent reduces the ill conditioning of the system. To compute converged weights to double precision, we use a multiprecision library that allows for computations in multiprecision arithmetic.

In the one-dimensional case we are able to show that the converged weights are the solution to a linear system of equations, where the system matrix is a Vandermonde matrix and where the right-hand side has an analytic expression in terms of the Riemann zeta function (see the Appendix). Hence, in this case, we can directly compute the converged weights by solving this system of equations.

The singularity corrections that we design are of order $\mathcal{O}(h^{2+\gamma+d+2p})$ in $\mathbb{R}^d$, $d = 1, 2$ as weights are modified at grid points in p layers around the singularity; see Theorem 3.7. In two dimensions ($\gamma = -1$), for $p = 0$, which corresponds to a single correction weight at the singularity, we have a third-order rule. For each additional layer of correction weights, the order of accuracy increases by 2. Compared with Aguilar & Chen (2002) our layers differ somewhat, with the number of correction weights in our approach growing more slowly as the number of layers is increased. We also have a theoretical analysis of the method's convergence rate.

In two dimensions, we have considered the singularity $1/|\mathbf{x}|$, which is the Green's function for the Laplace equation in three dimensions, instead of $\log(|\mathbf{x}|)$ as in Aguilar & Chen (2002) and Duan & Rokhlin (2009). A boundary integral equation for the three-dimensional Laplace equation contains integrals over two-dimensional surfaces that are the boundaries of the domain. This method would apply when the boundary is flat. Extensions based on the approach and the theory presented in this paper are discussed in the conclusions.

The outline of the paper is as follows. In Section 2, we describe the modified trapezoidal rules and their structure and we define the system of equations from which the correction weights can be obtained. The theoretical analysis is presented in Section 3, starting with the accuracy of the punctured trapezoidal rule, before we prove the accuracy of the modified trapezoidal rules. We also give a proof of convergence for the correction weights in one dimension. Numerical results to validate the constructed quadrature rules together with discussions concerning implementation aspects are provided in Section 4.

1.1 *Notation*

In order to render the text more legible, multiindex notation will be used. A multiindex in the d-dimensional set-up is $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_d)$. For $\boldsymbol{\alpha} \in \mathbb{R}^d, \mathbb{Z}^d$, including multiindices, we define the norms

$|\boldsymbol{\alpha}| = \sum_{i=1}^{d} |\alpha_i|$ and $|\boldsymbol{\alpha}|_2 = \sqrt{\sum_{i=1}^{d} \alpha_i^2}$. To be more explicit we write at times $|\boldsymbol{\alpha}|_1$ instead of $|\boldsymbol{\alpha}|$. We also use $\boldsymbol{\alpha}! = \alpha_1! \cdots \alpha_d!$. For $\mathbf{x} \in \mathbb{R}^d$ we define monomials $\mathbf{x}^{\boldsymbol{\alpha}} = x_1^{\alpha_1} \cdots x_d^{\alpha_d}$ and for the partial derivatives,

$$\partial^{\boldsymbol{\alpha}} f(\mathbf{x}) = \frac{\partial^{|\boldsymbol{\alpha}|}}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}} f(\mathbf{x}).$$

Occasionally, we will make use of the basis vectors in $\mathbb{R}^d$ which shall be denoted by $\mathbf{e}_i$ with $1 \leqslant i \leqslant d$.

The notation $[x]$ for the integer part of x and $\{x\}$ for the fractional part of x will also be used; recall that $x = [x] + \{x\}$. Throughout the manuscript C will denote a constant which is independent of other parameters relevant in the particular context where it is used, typically the grid spacing h and position $\mathbf{x}$. It may at times be accompanied by a numeric subscript to differentiate it from other similar constants.

1.2 *Trapezoidal rule*

Consider a function $f \in C^{2p+2}(\mathbb{R}^d)$, defined on the interval $S = [-a, a]$ for $d = 1$, and on the square $S = [-a, a]^2$ for $d = 2$. The standard trapezoidal rule in one dimension is then given by

$$\int_S f(x)\,\mathrm{d}x \approx T_h[f] := \sum_{\beta=-N}^{N} hf(\beta h) - \frac{1}{2}(hf(a) + hf(-a)), \quad h = a/N \tag{1.1}$$

and in two dimensions, with the same h, by

$$\int_S f(\mathbf{x})\,\mathrm{d}\mathbf{x} \approx T_h[f] := \sum_{\substack{\boldsymbol{\beta}h \in S \\ \boldsymbol{\beta} \in \mathbb{Z}^2}} h^2 f(\boldsymbol{\beta}h) - \frac{1}{2} \sum_{\substack{\boldsymbol{\beta}h \in \partial S \\ \boldsymbol{\beta} \in \mathbb{Z}^2}} h^2 f(\boldsymbol{\beta}h) - \frac{1}{4} \sum_{\substack{\boldsymbol{\beta}h \in \partial S_c \\ \boldsymbol{\beta} \in \mathbb{Z}^2}} h^2 f(\boldsymbol{\beta}h), \tag{1.2}$$

where we used ∂S_c to denote the four corner points of S. Typically, for a smooth integrand over a bounded interval, numerical integration using the trapezoidal rule exhibits second-order convergence. To delve further into the error analysis of the trapezoidal rule, and later the modified trapezoidal rule, we will use two main approaches: the Euler–Maclaurin expansion and Fourier analysis. We use the following precise form of the Euler–Maclaurin expansion.

THEOREM 1.1 (Euler–Maclaurin expansion) For a function $f \in C^{2p+2}([a, b])$,

$$\int_a^b f(x)\,\mathrm{d}x = T_h[f] + \sum_{\ell=1}^{p} \frac{h^{2\ell} b_{2\ell}}{(2\ell)!} (f^{(2\ell-1)}(b) - f^{(2\ell-1)}(a))$$
$$+ \frac{h^{2p+2}}{(2p+2)!} \int_a^b B_{2p+2}\left(\left\{\frac{x-a}{h}\right\}\right) f^{(2p+2)}(x)\,\mathrm{d}x. \tag{1.3}$$

The expression uses the Bernoulli polynomials B_p and the Bernoulli numbers defined as $b_p = B_p(0)$. The periodized versions $B_p(\{x\})$ are piecewise smooth and bounded functions detailed in Cohen (2007, Proposition 9.3.1 and Remark 2).

From the Euler–Maclaurin expansion (1.3) we see that there are two main sources of error in the trapezoidal rule, corresponding to the terms in the error expression. First, we have the contribution to the error from the boundaries given by

$$\sum_{\ell=1}^{p} \frac{h^{2\ell} b_{2\ell}}{(2\ell)!} (f^{(2\ell-1)}(b) - f^{(2\ell-1)}(a)). \tag{1.4}$$

Second, we have the contribution of the error which is determined by the regularity of the function,

$$\frac{h^{2p+2}}{(2p+2)!} \int_a^b B_{2p+2}\left(\left\{\frac{x-a}{h}\right\}\right) f^{(2p+2)}(x)\,\mathrm{d}x.$$

There are two common situations when the sum in (1.4) vanishes for integrands of class $C^{2p+2}(\mathbb{R})$: when the integrand is periodic on $[a,b]$ and when the integrand is compactly supported within (a,b). In this case the error of the trapezoidal rule is $\mathcal{O}(h^{2p+2})$. If the integrand is C^∞ and there are no boundary errors, the trapezoidal rule exhibits spectral convergence.

The accuracy of the trapezoidal rule may also be studied through Fourier analysis. In this approach we use the Poisson summation formula for $f \in C_c^2(\mathbb{R})$ and note that

$$T_h[f] = \sum_j hf(jh) = \sum_k \hat{f}\left(\frac{k}{h}\right) = \int f(x)\,\mathrm{d}x + \sum_{k\neq 0} \hat{f}\left(\frac{k}{h}\right),$$

where

$$\hat{f}(k) = \int f(x)\, e^{-2\pi \mathrm{i} kx}\,\mathrm{d}x. \tag{1.5}$$

Our aim is to show that this oscillatory integral can be estimated by

$$|\hat{f}(k)| \leqslant \frac{C}{|k|^p}, \quad p > 1,$$

from which it will then follow that

$$\left|T_h[f] - \int f(x)\,\mathrm{d}x\right| \leqslant \sum_{k\neq 0} \left|\hat{f}\left(\frac{k}{h}\right)\right| \leqslant Ch^p \sum_{k\neq 0} \frac{1}{|k|^p} \leqslant C'h^p.$$

2. Modified trapezoidal rules

We will construct modified trapezoidal rules with a singularity correction for functions with isolated singularities. More precisely, we consider functions $f(\mathbf{x}) = s(\mathbf{x})\phi(\mathbf{x})$ where $\phi(\mathbf{x})$ is regular and

$$s(\mathbf{x}) = |\mathbf{x}|^\gamma \quad \text{with} \begin{cases} \gamma \in (-1,0), & \mathbf{x} \in \mathbb{R}, \\ \gamma = -1, & \mathbf{x} \in \mathbb{R}^2. \end{cases} \tag{2.1}$$

2.1 *Simple correction*

Let us define the punctured trapezoidal rule, as applied to a compactly supported function f:

$$T_h^0[f] = \sum_{\boldsymbol{\beta} \neq 0} h^d f(\boldsymbol{\beta} h), \quad \boldsymbol{\beta} \in \mathbb{Z}^d. \tag{2.2}$$

Introduce the simply corrected quadrature rule $Q_h^0[\phi \cdot s] = T_h^0[\phi \cdot s] + a(h)\omega_0\phi(0)$, where $a(h)$ is a weight factor depending on the singularity and it is known beforehand. The correction weight $\omega_0(h)$ is defined by

$$a(h)\omega_0(h)g(0) = \int g(\mathbf{x})s(\mathbf{x})\,\mathrm{d}x - T_h^0[g \cdot s], \tag{2.3}$$

where $g(x)$ is a compactly supported function with $g(x) \neq 0$. The function $g(x)$ is introduced to annihilate the boundary errors from the punctured trapezoidal rule.

If the weight factor $a(h)$ is chosen correctly, then $\omega_0(h) \to \bar{\omega}_0$ as $h \to 0$ where $\bar{\omega}_0$ does not depend on h nor on g. The convergence rate of $\omega_0(h) \to \bar{\omega}_0$, however, depends strongly on the choice of g. Convergence is fast when the function g is *flat* at the singularity, i.e., it has several derivatives that vanish at the origin; see Section 4.

The modified quadrature rule reads

$$Q_h^0[\phi \cdot s] = T_h^0[\phi \cdot s] + a(h)\bar{\omega}_0\phi(0), \tag{2.4}$$

where for a space of dimension d,

$$a(h) = h^d s(h) = h^{\gamma+d}. \tag{2.5}$$

We will show below that adding a modification at the origin in this way will lead to a method of order $\mathcal{O}(h^{2+d+\gamma})$ for $s(\mathbf{x})$ given by (2.1). This assumes that the function $\phi(x)$ is regular enough, and also compactly supported within the integration domain. If it is not compactly supported, T_h^0 should be replaced by a boundary-corrected punctured trapezoidal rule (see Alpert, 1995).

2.2 *Higher-order correction*

A higher-order quadrature rule will involve more correction weights. Define

$$Q_h^p[\phi \cdot s] = T_h^0[\phi \cdot s] + a(h) \sum_{\boldsymbol{\beta} \in \mathcal{L}_p} \bar{\omega}_{\boldsymbol{\beta}}\phi(\boldsymbol{\beta} h), \tag{2.6}$$

where

$$\mathcal{L}_p = \{\boldsymbol{\beta} \in \mathbb{Z}^d \text{ s.t. } |\boldsymbol{\beta}|_1 \leqslant p\}. \tag{2.7}$$

In analogy with (2.3), the weights should satisfy the following equations:

$$\int g(\mathbf{x})s(\mathbf{x})\mathbf{x}^{2\boldsymbol{\alpha}}\,\mathrm{d}\mathbf{x} = T_h^0[g \cdot s \cdot \mathbf{x}^{2\boldsymbol{\alpha}}] + a(h) \sum_{\beta \in \mathcal{L}_p} \omega_{\boldsymbol{\beta}}(h)(\boldsymbol{\beta} h)^{2\boldsymbol{\alpha}} g(\boldsymbol{\beta} h) \quad \forall \boldsymbol{\alpha} \text{ s.t. } |\boldsymbol{\alpha}|_1 \leqslant p. \tag{2.8}$$

Temporarily denote the weight associated with a point (x_i, y_j) $(\beta = (i,j))$ by $w_{i,j}$. We then require $w_{\pm i,\pm j} = w_{\pm j,\pm i}$ for all possible combinations of signs. Such a weight will be denoted by w_q^m, where $q = |i| + |j|$, and m will be defined below. Due to these symmetry assumptions for the weights, the equations in (2.8) are stated only for even-order monomials since the equations for odd monomials

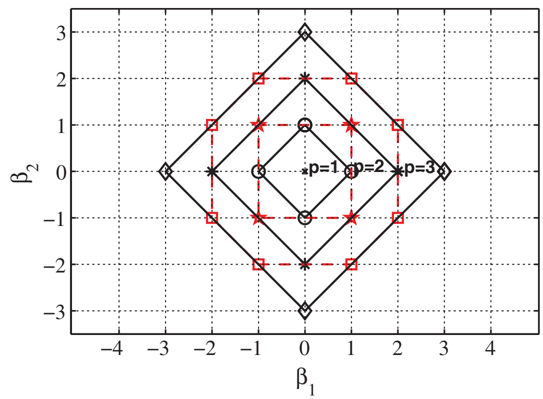

FIG. 1. The sets $\mathcal{L}_p$ include all grid points on and inside the layers indicated in the figure.

are automatically satisfied. We will show that the number of unknown weights equals the number of equations in (2.8).

Let us now consider the two-dimensional case. Consider sets $\mathcal{L}_p$ as in (2.7), with $d = 2$ (see Fig. 1). Introduce the subsets $\mathcal{G}_q^m \subset \mathcal{L}_p$ over which weights are equal,

$$\mathcal{G}_q^m = \{\boldsymbol{\beta} \in \mathbb{Z}^2 \text{ s.t. } |\boldsymbol{\beta}|_1 = q,\ |\boldsymbol{\beta}|_2 = \sqrt{m^2 + (q-m)^2}\}, \tag{2.9}$$

for $q = 0, \ldots, p$ and $m = 0, \ldots, [q/2]$. This defines disjoint subsets of $\mathcal{L}_p$ such that $\mathcal{G}_q^m \cap \mathcal{G}_{q'}^{m'} = 0$ for $m \neq m'$, or $q \neq q'$ and $\bigcup_{q \leqslant p} \bigcup_{m \leqslant [q/2]} \mathcal{G}_q^m = \mathcal{L}_p$.

To each of these sets $\mathcal{G}_q^m$ we associate one weight ω_q^m. The number of all distinct weights associated with $\mathcal{L}_p$ is

$$N_p = \sum_{m=0}^{p} ([m/2] + 1) = \begin{cases} (p/2)^2 + p + 1 & \text{if } p \text{ is even,} \\ (p+1)^2/4 + (p+1)/2 & \text{if } p \text{ is odd.} \end{cases} \tag{2.10}$$

We want to enforce (2.8) for all $\boldsymbol{\alpha}$ such that $|\boldsymbol{\alpha}| \leqslant p$. This set can be described by $\alpha \in \mathcal{M}_p$ with

$$\mathcal{M}_p = \bigcup_{q \leqslant p} \bigcup_{m \leqslant [q/2]} \{(q-m, m)\}. \tag{2.11}$$

For this set, we have $|\mathcal{M}_p| = N_p$, and (2.8) constitutes a square system. Relating to the notation above, we have $\boldsymbol{\alpha}_q^m = (q-m, m)$.

In Table 1 we list the monomials along with the sets of discretization points where the weights are corrected for layers up to $q = 4$. The first two columns provide the levels q and m at which we take a monomial $\mathbf{x}^{2\boldsymbol{\alpha}}$, where $\boldsymbol{\alpha} = \boldsymbol{\alpha}_q^m$ is listed in the third column. The last two columns list the sets of points, $\mathcal{G}_q^m$ and the associated weights $\bar{\omega}_q^m$.

Hence, we solve the following $N_p \times N_p$ linear system of equations:

$$a(h) \sum_{q=0}^{p} \sum_{m=0}^{[q/2]} \omega_q^m \sum_{\boldsymbol{\beta} \in \mathcal{G}_q^m} g(\boldsymbol{\beta} h)(\boldsymbol{\beta} h)^{2\boldsymbol{\alpha}} = \int g(\mathbf{x}) s(\mathbf{x}) \mathbf{x}^{2\boldsymbol{\alpha}}\, \mathrm{d}\mathbf{x} - T_h^0[g \cdot s \cdot \mathbf{x}^{2\boldsymbol{\alpha}}] \quad \forall \boldsymbol{\alpha} \in \mathcal{M}_p. \tag{2.12}$$

TABLE 1 *Sets of discrete points $\mathcal{G}_q^m$ for different values of q*

q	m	$\boldsymbol{\alpha}_q^m = (q-m, m)$	$\mathbf{x}^{2\boldsymbol{\alpha}}$	$\mathcal{G}_q^m$	Associated weight $\bar{\omega}_q^m$
0	0	(0,0)	1	$(0,0)$	$\bar{\omega}_0^0$
1	0	(1,0)	x_1^2	$(\pm 1, 0)\ (0, \pm 1)$	$\bar{\omega}_1^0$
2	0	(2,0)	x_1^4	$(\pm 2, 0)\ (0, \pm 2)$	$\bar{\omega}_2^0$
	1	(1,1)	$x_1^2 x_2^2$	$(\pm 1, \pm 1)$	$\bar{\omega}_2^1$
3	0	(3,0)	x_1^6	$(\pm 3, 0)\ (0, \pm 3)$	$\bar{\omega}_3^0$
	1	(2,1)	$x_1^4 x_2^2$	$(\pm 2, \pm 1)\ (\pm 1, \pm 2)$	$\bar{\omega}_3^1$
4	2	(2,2)	$x_1^4 x_2^4$	$(\pm 2, \pm 2)$	$\bar{\omega}_4^2$
	1	(3,1)	$x_1^6 x_2^2$	$(\pm 3, \pm 1)\ (\pm 1, \pm 3)$	$\bar{\omega}_4^1$
	0	(4,0)	x_1^8	$(\pm 4, 0)\ (0, \pm 4)$	$\bar{\omega}_4^0$
5	2	(3,2)	$x_1^6 x_2^4$	$(\pm 3, \pm 2)\ (\pm 2, \pm 3)$	$\bar{\omega}_5^2$
	1	(4,1)	$x_1^8 x_2^2$	$(\pm 4, \pm 1)\ (\pm 1, \pm 4)$	$\bar{\omega}_5^1$
	0	(5,0)	x_1^{10}	$(\pm 5, 0)\ (0, \pm 5)$	$\bar{\omega}_5^0$

In order to recast this system in matrix notation we introduce an index $i = 0, \ldots, N_p - 1$ and define $\boldsymbol{\alpha}_i$, ω_i and $\mathcal{G}_i$ from $\boldsymbol{\alpha}_q^m$, ω_q^m and $\mathcal{G}_q^m$, respectively, by letting $i = N_q + m$, where N_q is given by (2.10). We can then introduce the matrices $K,\ \tilde{I} \in \mathbb{R}^{N_p \times N_p}$ with elements

$$K_{ij} = \sum_{\boldsymbol{\beta} \in \mathcal{G}_j} \boldsymbol{\beta}^{2\boldsymbol{\alpha}_i}, \quad i, j = 0, \ldots, N_p - 1$$

and

$$\tilde{I}_{ij} = g(\boldsymbol{\beta} h)\delta_{ij}, \quad \boldsymbol{\beta} \in \mathcal{G}_j,\ i, j = 0, \ldots, N_p - 1,$$

which is well defined since the function $g(\boldsymbol{\beta} h)$ takes the same value for all $\boldsymbol{\beta} \in \mathcal{G}_i$.

The right-hand side of the system becomes

$$c_i(h) = \frac{1}{h^{2|\boldsymbol{\alpha}_i|} a(h)} \left(\int g(\mathbf{x}) s(\mathbf{x}) \mathbf{x}^{2\boldsymbol{\alpha}_i}\, \mathrm{d}\mathbf{x} - T_h^0[g \cdot s \cdot \mathbf{x}^{2\boldsymbol{\alpha}_i}] \right), \quad i = 0, \ldots, N_p - 1.$$

These expressions lead to the system

$$K\tilde{I}(h)\boldsymbol{\omega}(h) = \boldsymbol{c}(h). \tag{2.13}$$

Here, the solution vector $\boldsymbol{\omega}(h) = (\omega_0(h), \ldots, \omega_{N_p-1}(h))$ and the right-hand side $\boldsymbol{c}(h) = (c_0(h), \ldots, c_{N_p-1}(h))$ have the ordering provided by the new indexing.

For a given p consider the converged solution $\boldsymbol{\omega}(h) \to \bar{\boldsymbol{\omega}}$ of system (2.13) and define the modified quadrature rule for a singularity $s(\mathbf{x})$ with modified weights $\bar{\omega}_q^m$,

$$Q_h^p[\phi \cdot s] = T_h^0[\phi \cdot s] + A_h^p[\phi], \tag{2.14}$$

with

$$A_h^p[\phi] = a(h) \sum_{q=0}^{p} \sum_{m=0}^{[q/2]} \bar{\omega}_q^m \sum_{\boldsymbol{\beta} \in \mathcal{G}_q^m} \phi(\boldsymbol{\beta} h), \tag{2.15}$$

where $\mathcal{G}_q^m$ is as in (2.9). The constructed rule Q_h^p has accuracy $\mathcal{O}(h^{2p+3})$; see Theorem 3.7.

In one dimension the expressions for the sets $\mathcal{L}_p$, $\mathcal{M}_p$ greatly simplify since in this context $N_p = p+1$ and

$$\mathcal{L}_p = \{\beta \in \mathbb{Z}, |\beta| = j,\ j \leqslant p\}, \quad \mathcal{M}_p = \{\alpha \in \mathbb{N}, \alpha = j,\ j \leqslant p\}, \quad \mathcal{G}_i = \{\pm i\}.$$

So $K \in \mathbb{R}^{(p+1)\times(p+1)}$ has elements $K_{00} = 1$ and otherwise the Vandermonde structure $K_{ij} = 2j^{2i}$. Moreover, $\tilde{I}_{ij}(h) = g(ih)\delta_{ij}$. The right-hand-side entries are simply

$$c_i(h) := \frac{1}{h^{2i}a(h)} \left[\int g(x)s(x)x^{2i}\,\mathrm{d}x - T_h^0[g \cdot s \cdot x^{2i}] \right].$$

The corrected, punctured trapezoidal rule Q_h^p defined as in (2.14) has the correction operator

$$A_h^p[\phi] := a(h) \sum_{j=0}^{p} \bar{\omega}_j(\phi(jh) + \phi(-jh)). \tag{2.16}$$

3. Theoretical analysis

The techniques used to prove the accuracy of the modified quadrature rule differ in the one-dimensional set-up from the two-dimensional one. The Fourier approach is chosen for the lower dimension while in two dimensions the Euler–Maclaurin formula is applied in each direction. In this analysis, we focus on the errors due to the singularities and the accuracy of the singularity corrections. Therefore, we consider the integration of $f(x) = \phi(x)s(x)$, where $\phi(x)$ is compactly supported within the integration domain.

To begin with we provide an accuracy result for the punctured trapezoidal rule. Using this result we obtain an error estimate of the modified trapezoidal rule in terms of h and the difference $\boldsymbol{\omega}(h) - \bar{\boldsymbol{\omega}}$ in Theorem 3.7, where $\boldsymbol{\omega}(h) - \bar{\boldsymbol{\omega}}$ can be made sufficiently small with a proper choice of g so that it does not alter the asymptotic order. This is proved in the one-dimensional case, where we show that $\boldsymbol{\omega}(h) \to \bar{\boldsymbol{\omega}}$ and also obtain an estimate of $|\boldsymbol{\omega}(h) - \bar{\boldsymbol{\omega}}|$, thus yielding a complete error estimate for the modified trapezoidal rule in one dimension. In two dimensions, we offer no rigorous proofs for the convergence of the weights, but note the same behaviour as in one dimension in numerical experiments.

3.1 *Accuracy of the punctured trapezoidal rule*

To prove the order of convergence of the constructed quadrature rule we start by deriving an error estimate for the punctured trapezoidal rule. Theorem 3.1 states the one-dimensional result. The corresponding two-dimensional result in Theorem 3.2 is weaker; note that the function $f = \tilde{g} \cdot s$ vanishes at the origin, thus $\mathcal{T}_h[f] = \mathcal{T}_h^0[f]$. General error estimates of the type below were derived in Lyness (1976). However, those also include the boundary errors and do not cover the cases we are interested in here.

THEOREM 3.1 Consider $f:\mathbb{R}\to\mathbb{R}$ given as $f=g(x)s(x)$ where $s(x)=|x|^{\gamma}$ with $\gamma>-1$. Let p and q be integers such that $0\leqslant p<q$ and $2q+1>\gamma$. Take $g(x)\in C_c^{2q+2}(\mathbb{R})$ with $g^{(k)}(0)=0$ for $k=2,4,\ldots,2p$. Then

$$\left|\int f(x)\,\mathrm{d}x - T_h^0[f] - g(0)h^{\gamma+1}\bar{c}(\gamma)\right| \leqslant C(h^{2p+\gamma+3}+h^{2q+2}),$$

where $\bar{c}(\gamma)$ depends on γ but is independent of h and g.

We note that if $\gamma>0$ this also gives an estimate for the standard trapezoidal rule since then $f(0)=0$ and $T_h[f]=T_h^0[f]$. The proof of this theorem is given in Section 3.1.1. In Lemma A2 in the Appendix, a closed form expression for $\bar{c}(\gamma)$ is given.

THEOREM 3.2 Consider $f:\mathbb{R}^2\to\mathbb{R}$ given as $f(\mathbf{x})=\tilde{g}(\mathbf{x})s(\mathbf{x})$ where $s(\mathbf{x})=1/|\mathbf{x}|$. Let q and p be integers such that $q>p$. Take $\tilde{g}\in C_c^{2q+3}(\mathbb{R}^2)$ with $\partial^{\boldsymbol{k}}\tilde{g}(\mathbf{0})=0$ for all $\boldsymbol{k}\in\mathbb{N}^2$ such that $|\boldsymbol{k}|<2p+2$. Then it holds that

$$\left|\int f(\mathbf{x})\,\mathrm{d}\mathbf{x} - \mathcal{T}_h[f]\right| \leqslant Ch^{2p+3}.$$

This theorem is proved in Section 3.1.2.

3.1.1 *One-dimensional case* In this section we prove Theorem 3.1. We begin by introducing a cut-off function $\psi\in C^{\infty}$ satisfying $\psi(x)=\psi(-x)$ and

$$\psi(x)=\begin{cases}0, & |x|\leqslant\frac{1}{2},\\ 1, & |x|\geqslant 1.\end{cases} \tag{3.1}$$

We then have

$$T_h^0[f]=T_h[f\psi(\cdot/h)].$$

Consequently,

$$\int f(x)\,\mathrm{d}x - T_h^0[f] = \int f(x)(1-\psi(x/h))\,\mathrm{d}x + \int f(x)\psi(x/h)\,\mathrm{d}x - T_h[f\psi(\cdot/h)], \tag{3.2}$$

and we can estimate the two parts separately. For the first term we have

$$\begin{aligned}\int f(x)(1-\psi(x/h))\,\mathrm{d}x &= \int_{-h}^{h} g(x)s(x)(1-\psi(x/h))\,\mathrm{d}x\\ &= h^{\gamma+1}\int_{-1}^{1} g(hx)s(x)(1-\psi(x))\,\mathrm{d}x,\end{aligned} \tag{3.3}$$

where we have used the definition of ψ in (3.1) and a rescaling of the interval. By the symmetry of $\psi(x)$ and $s(x)$ and the assumption of vanishing derivatives,

$$\int_{-1}^{1}(g(hx)-g(0))s(x)(1-\psi(x))\,\mathrm{d}x = \int_{-1}^{1}\left(g(hx)-\sum_{j=0}^{2p+1}\frac{g^{(j)}(0)}{j!}(hx)^j\right)s(x)(1-\psi(x))\,\mathrm{d}x.$$

Therefore, after estimating the remainder term in the Taylor expansion of $g(x)$, which is bounded by $\tilde{C}h^{2p+2}|x|^{2p+2}$,

$$\left|\int_{-1}^{1}(g(hx)-g(0))s(x)(1-\psi(x))\,\mathrm{d}x\right| \leqslant \tilde{C}h^{2p+2}\int_{-1}^{1}|x|^{\gamma+2p+2}|1-\psi(x)|\,\mathrm{d}x \leqslant Ch^{2p+2}. \tag{3.4}$$

Define

$$\bar{c}_1(\gamma)=\int_{-1}^{1}s(x)(1-\psi(x))\,\mathrm{d}x.$$

Then we obtain from (3.4) and (3.3),

$$\begin{aligned}\left|\int f(x)(1-\psi(x))\,\mathrm{d}x-g(0)h^{\gamma+1}\bar{c}_1(\gamma)\right| &= h^{\gamma+1}\left|\int_{-1}^{1}(g(hx)-g(0))s(x)(1-\psi(x))\,\mathrm{d}x\right| \\ &\leqslant Ch^{2p+\gamma+3}.\end{aligned} \tag{3.5}$$

For the second term in (3.2) we can use the strategy based on the Fourier analysis as in Section 1.2 for the standard trapezoidal rule applied to $f(x)\psi(x/h)$. Hence, since $f(x)\psi(x/h)\in C_c^{2q+2}(\mathbb{R})$ we obtain from the Poisson summation formula (1.5),

$$\begin{aligned}T_h[f\psi(\cdot/h)] &= \int f(x)\psi(x/h)\,\mathrm{d}x+\sum_{k\neq 0}\hat{f}_\psi(k/h,h), \\ \hat{f}_\psi(k,h) &= \int f(x)\psi(x/h)\,e^{-2\pi \mathrm{i}kx/h}\,\mathrm{d}x.\end{aligned} \tag{3.6}$$

Moreover, by the symmetry of $\psi(x)$,

$$\begin{aligned}\hat{f}_\psi(k/h,h)+\hat{f}_\psi(-k/h,h) &= 2\int g(x)s(x)\psi(x/h)\cos(2\pi kx/h)\,\mathrm{d}x \\ &= 2\Re\int_0^{\infty}(g(x)+g(-x))s(x)\psi(x/h)\,e^{2\pi \mathrm{i}kx/h}\,\mathrm{d}x.\end{aligned} \tag{3.7}$$

We will now use Lemma 3.3 stated and proved below, which provides estimates on oscillatory integrals of this type. Since the even derivatives of $g(x)$ are zero up to order $2p$ at $x=0$, all derivatives of $\tilde{g}(x)=g(x)+g(-x)$ are zero up to order $2p+1$ at $x=0$. We can therefore apply Lemma 3.3 to the integral with $2p+1$ for p and $2q+2$ for q. We obtain

$$\begin{aligned}\int_0^{\infty}(g(x)+g(-x))s(x)\psi(x/h)\,e^{2\pi \mathrm{i}kx/h}\,\mathrm{d}x &= \tilde{g}(0)W(2\pi k)h^{\gamma+1}(2\pi k)^{-2(q+1)} \\ &\quad+\mathcal{O}(k^{-2(q+1)}(h^{\gamma+2p+3}+h^{2q+2})).\end{aligned} \tag{3.8}$$

Using (3.7) combined with (3.8), an expression for $\hat{f}_\psi(k/h,h) + \hat{f}_\psi(-k/h,h)$ is obtained. Rewriting the sum in (3.6) to use this expression, we get

$$\begin{aligned}
T_h[f\psi(\cdot/h)] &= \int f(x)\psi(x/h)\,\mathrm{d}x + 2\Re\sum_{k=1}^{\infty}\int_0^{\infty}(g(x)+g(-x))s(x)\psi(x/h)\,e^{2\pi\mathrm{i}kx/h}\,\mathrm{d}x \\
&= \int f(x)\psi(x/h)\,\mathrm{d}x + 4g(0)h^{\gamma+1}\Re\sum_{k=1}^{\infty}\frac{W(2\pi k)}{(2\pi k)^{2(q+1)}} \\
&\quad + [h^{\gamma+2p+3}+h^{2q+2}]\sum_{k=1}^{\infty}\mathcal{O}(k^{-2(q+1)}) \\
&= \int f(x)\psi(x/h)\,\mathrm{d}x + g(0)h^{\gamma+1}\bar{c}_2(\gamma) + \mathcal{O}(h^{\gamma+2p+3}+h^{2q+2}),
\end{aligned} \tag{3.9}$$

where

$$\bar{c}_2(\gamma) = 4\Re\sum_{k=1}^{\infty}\frac{W(2\pi k)}{(2\pi k)^{2(q+1)}}.$$

Note that this is well defined since $q \geqslant 0$ and $W(k)$ is bounded in k. Using (3.2) we get

$$\begin{aligned}
&\left|\int f(x)\,\mathrm{d}x - T_h^0(f) - g(0)h^{\gamma+1}(\bar{c}_1(\gamma)-\bar{c}_2(\gamma))\right| \\
&\quad\leqslant \left|\int f(x)(1-\psi(x/h))\,\mathrm{d}x - g(0)h^{\gamma+1}\bar{c}_1(\gamma)\right| \\
&\qquad + \left|\int f(x)\psi(x/h)\,\mathrm{d}x - T_h(f\psi(\cdot/h)) + g(0)h^{\gamma+1}\bar{c}_2(\gamma)\right|.
\end{aligned}$$

The result of Theorem 3.1 now follows from (3.5) and (3.9) with

$$\bar{c}(\gamma) = \bar{c}_1(\gamma) - \bar{c}_2(\gamma) = \int_{-1}^{1} s(x)(1-\psi(x))\,\mathrm{d}x - 4\Re\sum_{k=1}^{\infty}\frac{W(2\pi k)}{(2\pi k)^{2(q+1)}},$$

which is independent of h and $g(x)$. It remains to state and prove Lemma 3.3.

Lemma 3.3 Let p and q be integers such that $0 \leqslant p < q$ and h and k are positive real numbers, and γ be any real number. Suppose $g(x) \in C_c^q$ with supp $g \subset [0,L]$ and $g^{(\ell)}(0) = 0$ for $\ell = 1,\ldots,p$. If $q > \gamma+1$ and $\psi(x)$ is as given in (3.1), then there is a function $W(k)$ such that

$$\left|\int_0^{\infty}\psi(x/h)g(x)x^{\gamma}\,e^{\mathrm{i}kx/h}\,\mathrm{d}x - g(0)W(k)h^{\gamma+1}k^{-q}\right| \leqslant C_q k^{-q}(h^{\gamma+2+p}+h^q), \tag{3.10}$$

where $W(k)$ is bounded in k and independent of h and $g(x)$ (but depends on q).

Proof. We let $s(x) = x^\gamma$ and note that $|s^{(j)}(x)| \leqslant Cx^{\gamma-j}$. Since supp $\psi(x/h)g(x) \subset [h/2, L] \subset (0, \infty)$ we have, after q integrations by parts,

$$I(h,k) := \int_0^\infty \psi(x/h)g(x)s(x)\, e^{\mathrm{i}kx/h}\, \mathrm{d}x = \left(\frac{\mathrm{i}h}{k}\right)^q \int_0^\infty \left(\frac{\mathrm{d}^q}{\mathrm{d}x^q}\psi(x/h)g(x)s(x)\right) e^{\mathrm{i}kx/h}\, \mathrm{d}x.$$

Define $W(k)$ as

$$W(k) = \mathrm{i}^q \int_0^\infty \left(\frac{\mathrm{d}^q}{\mathrm{d}x^q}\psi(x)s(x)\right) e^{\mathrm{i}kx}\, \mathrm{d}x. \tag{3.11}$$

Clearly, $W(k)$ does not depend on h. Moreover, $\psi^{(j)}(x)$ is compactly supported for $j \geqslant 1$ and $|s^{(q)}(x)| \leqslant x^{\gamma-q}$ is integrable because $q > \gamma + 1$. Therefore,

$$|W(k)| \leqslant \int_0^\infty |\psi(x)s^{(q)}(x)|\, \mathrm{d}x + \sum_{j=1}^{q} d_{q,j} \int_0^\infty |\psi^{(j)}(x)s^{(q-j)}(x)|\, \mathrm{d}x \leqslant C,$$

where $d_{q,j}$ are the binomial coefficients. The estimate is independent of k, showing the boundedness of $W(k)$. After rescaling the integral we also have

$$\begin{aligned} W(k) &= \mathrm{i}^q h^{q-1} \int_0^\infty \left(\frac{\mathrm{d}^q}{\mathrm{d}x^q}\psi(x/h)s(x/h)\right) e^{\mathrm{i}kx/h}\, \mathrm{d}x \\ &= \mathrm{i}^q h^{q-1-\gamma} \int_0^\infty \left(\frac{\mathrm{d}^q}{\mathrm{d}x^q}\psi(x/h)s(x)\right) e^{\mathrm{i}kx/h}\, \mathrm{d}x. \end{aligned}$$

Then, with $r(x) := \psi(x/h)g(x)$,

$$\begin{aligned} &I(h,k) - g(0)W(k)h^{\gamma+1}k^{-q} \\ &\quad = \left(\frac{\mathrm{i}h}{k}\right)^q \int_0^\infty \left(\frac{\mathrm{d}^q}{\mathrm{d}x^q}[r(x) - g(0)\psi(x/h)]s(x)\right) e^{\mathrm{i}kx/h}\, \mathrm{d}x \\ &\quad = \left(\frac{h}{\mathrm{i}k}\right)^q \sum_{j=0}^{q} d_{q,j} \int_0^\infty [r^{(j)}(x) - g(0)h^{-j}\psi^{(j)}(x/h)]s^{(q-j)}(x)\, e^{\mathrm{i}kx/h}\, \mathrm{d}x. \end{aligned} \tag{3.12}$$

We have the following expression for the derivatives of $r(x)$:

$$r^{(j)}(x) = \begin{cases} \displaystyle\sum_{\ell=0}^{j} \frac{d_{j,\ell}}{h^{j-\ell}} \psi^{(j-\ell)}(x/h)g^{(\ell)}(x), & h/2 \leqslant x \leqslant h, \\ g^{(j)}(x), & h < x \leqslant L, \end{cases}$$

since $\psi^{(j)}(x) \equiv 0$ for $j > 0$ and $x > h$. Let $\delta_{i,j}$ be the Kronecker delta. Exploiting the facts that $\psi(x/h) \equiv 0$ for $x < h/2$ and $\psi(x/h) \equiv 1$ for $x > h$ we obtain, for $0 \leqslant j \leqslant q$,

$$\begin{aligned}
&\int_0^\infty [r^{(j)}(x) - g(0)h^{-j}\psi^{(j)}(x/h)]s^{(q-j)}(x)\, e^{\mathrm{i}kx/h}\,\mathrm{d}x \\
&\quad = \int_{h/2}^h \left[\sum_{\ell=0}^{j} \frac{d_{j,\ell}}{h^{j-\ell}}\psi^{(j-\ell)}(x/h)g^{(\ell)}(x) - \frac{1}{h^j}\psi^{(j)}(x/h)g(0)\right] s^{(q-j)}(x)\, e^{\mathrm{i}kx/h}\,\mathrm{d}x \\
&\qquad + \int_h^L g^{(j)}(x)s^{(q-j)}(x)\, e^{\mathrm{i}kx/h}\,\mathrm{d}x - \delta_{0,j}g(0)\int_h^\infty s^{(q)}(x)\, e^{\mathrm{i}kx/h}\,\mathrm{d}x \\
&\quad = \sum_{\ell=0}^{j} \frac{d_{j,\ell}}{h^{j-\ell}} \int_{h/2}^h \psi^{(j-\ell)}(x/h)[g^{(\ell)}(x) - \delta_{0,\ell}g(0)]s^{(q-j)}(x)\, e^{\mathrm{i}kx/h}\,\mathrm{d}x \\
&\qquad + \int_h^L [g^{(j)}(x) - \delta_{0,j}g(0)]s^{(q-j)}(x)\, e^{\mathrm{i}kx/h}\,\mathrm{d}x \\
&\qquad - \delta_{0,j}g(0)\int_L^\infty s^{(q)}(x)\, e^{\mathrm{i}kx/h}\,\mathrm{d}x. \qquad (3.13)
\end{aligned}$$

We will now use the assumption that $g^{(\ell)}(0) = 0$ for $1 \leqslant \ell \leqslant p$. From Taylor's theorem we get

$$|g^{(j)}(x) - g^{(j)}(0)| \leqslant |g^{(p+1)}|_\infty \frac{|x|^{p+1-j}}{(p+1-j)!} = C|x|^{p+1-j}, \quad 0 \leqslant j \leqslant p,$$

and therefore also

$$|g^{(j)}(x) - \delta_{0,j}g(0)| \leqslant Cx^{\max(p+1-j,0)}.$$

We use this to estimate the integrals in (3.13). First, for $0 \leqslant j \leqslant q$ and $0 \leqslant \ell \leqslant j$,

$$\begin{aligned}
&\frac{1}{h^{j-\ell}}\left|\int_{h/2}^h \psi^{(j-\ell)}(x/h)[g^{(\ell)}(x) - \delta_{0,\ell}g(0)]s^{(q-j)}(x)\, e^{\mathrm{i}kx/h}\,\mathrm{d}x\right| \\
&\quad \leqslant \frac{C}{h^{j-\ell}}\int_{h/2}^h x^{\max(p+1-\ell,0)+\gamma-q+j}\,\mathrm{d}x \leqslant Ch^{\max(p+1-\ell,0)+\gamma-q+1+\ell} \\
&\quad \leqslant Ch^{p+2+\gamma-q},
\end{aligned}$$

where we used the fact that $h^{\max(r,0)} \leqslant h^r$ when $h < 1$. Moreover, for the second integral in (3.13),

$$\begin{aligned}
&\left|\int_h^L [g^{(j)}(x) - \delta_{0,j}g(0)]s^{(q-j)}(x)\, e^{\mathrm{i}kx/h}\,\mathrm{d}x\right| \\
&\quad \leqslant C\int_h^L x^{\max(p+1-j,0)+\gamma-q+j}\,\mathrm{d}x \leqslant C(h^{\max(p+1-j,0)+\gamma-q+j+1} + 1) \\
&\quad \leqslant C(h^{p+2+\gamma-q} + 1).
\end{aligned}$$

Finally, for the last integral in (3.13),

$$\left|\int_L^\infty s^{(q)}(x)\, e^{\mathrm{i}kx/h}\, \mathrm{d}x\right| \leqslant C\int_L^\infty x^{\gamma-q}\, \mathrm{d}x \leqslant C,$$

since $q>\gamma+1$. Together with (3.12) these estimates show that

$$|I(h,k)-g(0)W(k)h^{\gamma+1}k^{-q}| \leqslant C\left(\frac{h}{k}\right)^q (h^{p+2+\gamma-q}+1) \leqslant Ck^{-q}(h^{\gamma+2+p}+h^q).$$

This proves the lemma. □

3.1.2 *Two-dimensional case* The Euler–Maclaurin expansion formula is the basis for the theoretical analysis in two dimensions. Since it provides an error estimate based on the cancellation and boundedness of higher-order derivatives—see (1.1)—we first evaluate the higher-order derivatives of the singular function $s(\mathbf{x})=1/|\mathbf{x}|$. The concluding result of this subsection is the proof of Theorem 3.2.

LEMMA 3.4 The partial derivatives of order $\boldsymbol{k}$ of $\mathbf{x}^{\boldsymbol{\alpha}}/|\mathbf{x}|$ with $\mathbf{x}=(x_1,x_2)$ are given as

$$\partial^{\boldsymbol{k}}\frac{\mathbf{x}^{\boldsymbol{\alpha}}}{|\mathbf{x}|} = \frac{1}{|\mathbf{x}|^{|\boldsymbol{k}|-|\boldsymbol{\alpha}|+1}} P_{\boldsymbol{k},\boldsymbol{\alpha}}\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right), \tag{3.14}$$

where $P_{\boldsymbol{k},\boldsymbol{\alpha}}$ is a polynomial with $\deg P_{\boldsymbol{k},\boldsymbol{\alpha}} = |\boldsymbol{k}|+|\boldsymbol{\alpha}|$ in two variables $P_{\boldsymbol{k},\boldsymbol{\alpha}}(\mathbf{x}) = P_{\boldsymbol{k},\boldsymbol{\alpha}}(x_1,x_2)$.

Proof. For $\boldsymbol{k}=(0,0)$ we have

$$\partial^{\boldsymbol{k}}\frac{\mathbf{x}^{\boldsymbol{\alpha}}}{|\mathbf{x}|} = \left(\frac{\mathbf{x}}{|\mathbf{x}|}\right)^{\boldsymbol{\alpha}}\frac{1}{|\mathbf{x}|^{1-|\boldsymbol{\alpha}|}},$$

which agrees with (3.14) with $P_{\boldsymbol{k},\boldsymbol{\alpha}}(\mathbf{z})=\mathbf{z}^{\boldsymbol{\alpha}}$. We let $P^{(j)}_{\boldsymbol{k},\boldsymbol{\alpha}}(x_1,x_2) := \partial_{x_j}P_{\boldsymbol{k},\boldsymbol{\alpha}}(x_1,x_2)$ and note that these are polynomials of degree one less than the degree of $P_{\boldsymbol{k},\boldsymbol{\alpha}}(x_1,x_2)$ itself. Assume that the theorem statement is true for $\boldsymbol{k}$ and let $\boldsymbol{k}\to\boldsymbol{k}+\mathbf{e}_1$. Then we want to show that

$$\partial^{\boldsymbol{k}+\boldsymbol{e}_1}\frac{\mathbf{x}^{\boldsymbol{\alpha}}}{|\mathbf{x}|} = \frac{1}{|\mathbf{x}|^{|\boldsymbol{k}|-|\boldsymbol{\alpha}|+2}} P_{\boldsymbol{k}+\boldsymbol{e}_1,\boldsymbol{\alpha}}\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right),$$

for some polynomial $P_{\boldsymbol{k}+\boldsymbol{e}_1,\boldsymbol{\alpha}}$ of degree $|\boldsymbol{k}|+|\boldsymbol{\alpha}|+1$. By applying the chain rule and evaluating, we get

$$\begin{aligned}
\partial_{x_1}\frac{1}{|\mathbf{x}|^{|\boldsymbol{k}|-|\boldsymbol{\alpha}|+1}}P_{\boldsymbol{k},\boldsymbol{\alpha}}\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right) &= P_{\boldsymbol{k},\boldsymbol{\alpha}}\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right)\partial_{x_1}\frac{1}{|\mathbf{x}|^{|\boldsymbol{k}|-|\boldsymbol{\alpha}|+1}} \\
&\quad + \frac{1}{|\mathbf{x}|^{|\boldsymbol{k}|-|\boldsymbol{\alpha}|+1}}\left(\left(\frac{1}{|\mathbf{x}|}-\frac{x_1^2}{|\mathbf{x}|^3}\right)P^{(1)}_{\boldsymbol{k},\boldsymbol{\alpha}}\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right)+\left(\frac{x_1x_2}{|\mathbf{x}|^3}\right)P^{(2)}_{\boldsymbol{k},\boldsymbol{\alpha}}\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right)\right) \\
&= \frac{-(|\boldsymbol{k}|-|\boldsymbol{\alpha}|+1)x_1}{|\mathbf{x}|^{|\boldsymbol{k}|-|\boldsymbol{\alpha}|+3}}P_{\boldsymbol{k},\boldsymbol{\alpha}}\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right)
\end{aligned}$$

$$+\frac{1}{|\mathbf{x}|^{|\boldsymbol{k}|-|\boldsymbol{\alpha}|+2}}\left(\left(1-\frac{x_1^2}{|\mathbf{x}|^2}\right)P^{(1)}_{\boldsymbol{k},\boldsymbol{\alpha}}\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right)+\left(\frac{x_1x_2}{|\mathbf{x}|^2}\right)P^{(2)}_{\boldsymbol{k},\boldsymbol{\alpha}}\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right)\right)$$
$$=:\frac{1}{|\mathbf{x}|^{|\boldsymbol{k}|-|\boldsymbol{\alpha}|+2}}P_{\boldsymbol{k}+\mathbf{e}_1,\boldsymbol{\alpha}}\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right),$$

where $\deg P_{\boldsymbol{k}+\mathbf{e}_1,\boldsymbol{\alpha}}=|\boldsymbol{k}|+|\boldsymbol{\alpha}|+1$, which is what we needed to show. The case $\boldsymbol{k}\to\boldsymbol{k}+\mathbf{e}_2$ can be proved in the same way. This induction step proves that the expression provided by the lemma is valid. □

LEMMA 3.5 Let $\Omega\subset\mathbb{R}^2$ be a compact set. Consider $f:\Omega\to\mathbb{R}$ given as $f(\mathbf{x})=\tilde{g}(\mathbf{x})\cdot s(\mathbf{x})$ where $s(\mathbf{x})=1/|\mathbf{x}|$ and $\tilde{g}\in C^q(\Omega)$ has vanishing derivatives up to order $p\leqslant q$ at the origin: $\partial^{\boldsymbol{k}}\tilde{g}(\mathbf{0})=0$ for all $\boldsymbol{k}\in\mathbb{N}^2$ such that $|\boldsymbol{k}|<p$. Then, for each $|\boldsymbol{n}|\leqslant q$ there is a constant $C(\boldsymbol{n})$ independent of $\mathbf{x}$ and p, such that
$$|\partial^{\boldsymbol{n}}f(\mathbf{x})|\leqslant C(\boldsymbol{n})|\mathbf{x}|^{p-1-|\boldsymbol{n}|}\quad\forall\mathbf{x}\in\Omega\setminus\{0\}.$$

Proof. In order to compute the higher-order derivatives of f the Leibniz rule is applied:

$$\partial^{\boldsymbol{n}}(f(\mathbf{x}))=\partial^{\boldsymbol{n}}(\tilde{g}(\mathbf{x})\cdot s(\mathbf{x}))=\sum_{\boldsymbol{\ell}+\boldsymbol{r}=\boldsymbol{n}}b^n_{\ell r}\partial^{\boldsymbol{\ell}}\tilde{g}(\mathbf{x})\partial^{\boldsymbol{r}}s(\mathbf{x}),$$

where $b^n_{\ell r}$ are binomial coefficients. By Taylor expanding $\partial^{\boldsymbol{\ell}}\tilde{g}$ and recalling that $\partial^{\boldsymbol{k}}\tilde{g}(\mathbf{0})=0$ for all $\boldsymbol{k}\in\mathbb{N}^2$ such that $|\boldsymbol{k}|<p$, we have, for $|\boldsymbol{\ell}|<p$,

$$\partial^{\boldsymbol{\ell}}\tilde{g}(\mathbf{x})=\sum_{|\boldsymbol{k}|=0}^{p-1-|\boldsymbol{\ell}|}\frac{\mathbf{x}^{\boldsymbol{k}}}{\boldsymbol{k}!}\frac{\partial^{(\boldsymbol{\ell}+\boldsymbol{k})}\tilde{g}(\mathbf{0})}{\partial\mathbf{x}^{\boldsymbol{k}}}+R_\ell(\mathbf{x})|\mathbf{x}|^{p-|\boldsymbol{\ell}|}=R_\ell(\mathbf{x})|\mathbf{x}|^{p-|\boldsymbol{\ell}|}.$$

On the other hand, when $p\leqslant|\boldsymbol{\ell}|\leqslant q$ we just use the boundedness of $\partial^{\boldsymbol{\ell}}\tilde{g}$ over Ω and obtain, for all $\mathbf{x}\in\Omega$,

$$|\partial^{\boldsymbol{\ell}}\tilde{g}(\mathbf{x})|\leqslant C_0\begin{cases}|\mathbf{x}|^{p-|\boldsymbol{\ell}|}, & |\boldsymbol{\ell}|<p,\\ 1, & p\leqslant|\boldsymbol{\ell}|\leqslant q,\end{cases}\qquad C_0=\max_{|\ell|\leqslant|n|}\sup_{x\in\Omega}\max(|R_\ell(\mathbf{x})|,|\partial^{\boldsymbol{\ell}}\tilde{g}(\mathbf{x})|).$$

By using Lemma 3.4 with $\boldsymbol{\alpha}=0$ for $\partial^{\boldsymbol{r}}s(\mathbf{x})$ we have, for $\boldsymbol{r}\leqslant\boldsymbol{n}$,

$$|\partial^{\boldsymbol{r}}s(\mathbf{x})|=\frac{1}{|\mathbf{x}|^{|\boldsymbol{r}|+1}}P_{\boldsymbol{r},0}\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right)\leqslant\frac{C_1}{|\mathbf{x}|^{|\boldsymbol{r}|+1}},\qquad C_1=\max_{|r|\leqslant|n|}\sup_{x}\left|P_{\boldsymbol{r},0}\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right)\right|,$$

where C_1 is bounded since $\{\mathbf{x}/|\mathbf{x}|,\ \mathbf{x}\in\mathbb{R}^2\}$ is compact. Together these estimates yield

$$\begin{aligned}|\partial^{\boldsymbol{n}}(f(\mathbf{x}))|&\leqslant\sum_{\boldsymbol{\ell}+\boldsymbol{r}=\boldsymbol{n}}b^n_{\ell r}|\partial^{\boldsymbol{\ell}}\tilde{g}(\mathbf{x})||\partial^{\boldsymbol{r}}s(\mathbf{x})|\\
&\leqslant C_0C_1\sum_{\boldsymbol{\ell}+\boldsymbol{r}=\boldsymbol{n}}\frac{b^n_{\ell r}}{|\mathbf{x}|^{|\boldsymbol{r}|+1}}\begin{cases}|\mathbf{x}|^{p-|\boldsymbol{\ell}|}, & |\boldsymbol{\ell}|<p,\\ 1, & p\leqslant|\boldsymbol{\ell}|\leqslant q,\end{cases}\\
&=C_0C_1\sum_{\boldsymbol{\ell}+\boldsymbol{r}=\boldsymbol{n}}b^n_{\ell r}\begin{cases}|\mathbf{x}|^{p-1-|\boldsymbol{n}|}, & |\boldsymbol{\ell}|<p,\\ |\mathbf{x}|^{-|\boldsymbol{r}|-1}, & p\leqslant|\boldsymbol{\ell}|\leqslant q.\end{cases}\end{aligned}\tag{3.15}$$

Let $\eta := \sup_{x\in\Omega} |\mathbf{x}|$. Then, when $p \leqslant |\boldsymbol{\ell}| \leqslant |\boldsymbol{n}| \leqslant q$,

$$\max_{\ell+r=n} |\mathbf{x}|^{-|\boldsymbol{r}|-1} = \max_{\ell+r=n} \frac{1}{\eta^{|\boldsymbol{r}|+1}} \left|\frac{\mathbf{x}}{\eta}\right|^{-|\boldsymbol{r}|-1}$$
$$\leqslant \left(\max_{\ell+r=n} \frac{1}{\eta^{|\boldsymbol{r}|+1}}\right) \left|\frac{\mathbf{x}}{\eta}\right|^{p-1-|\boldsymbol{n}|} =: C_2|\mathbf{x}|^{p-1-|\boldsymbol{n}|}.$$

Entering this in (3.15) we finally have

$$|\partial^{\boldsymbol{n}}(f(\mathbf{x}))| \leqslant |\mathbf{x}|^{p-1-|\boldsymbol{n}|} C_0 C_1 \sum_{\boldsymbol{\ell}+\boldsymbol{r}=\boldsymbol{n}} b^n_{\ell r}(1+C_2),$$

which proves the lemma since the sum is bounded independently of p. □

LEMMA 3.6 Consider $f:\mathbb{R}^2 \to \mathbb{R}$ given as $f(\mathbf{x}) = \tilde{g}(\mathbf{x}) \cdot s(\mathbf{x})$ where $s(\mathbf{x}) = 1/|\mathbf{x}|$. Take $\tilde{g} \in C_c^{2m+3}(\mathbb{R}^2)$ with $\partial^{\boldsymbol{k}}\tilde{g}(\mathbf{0}) = 0$ for all $\boldsymbol{k} \in \mathbb{N}^2$ such that $|\boldsymbol{k}| < 2p+2$. Then

$$\int_{-a}^{a} |\partial^{\boldsymbol{n}}(\tilde{g}(\mathbf{x})s(\mathbf{x}))|\,\mathrm{d}x_1 \leqslant C|x_2|^{2p-2m}, \quad |\boldsymbol{n}| = 2m+2,$$

with $\mathbf{x} = (x_1, x_2)$, $x_2 \neq 0$, when $m > p$. This estimate is also true when $m = p$ if $\mathbf{n}$ contains at least one derivative in the x_1 direction, i.e., if we can write $\mathbf{n} = \tilde{\mathbf{n}} + \mathbf{e}_1$ for some multiindex $\tilde{\mathbf{n}}$.

Proof. We first consider the case $m > p$. By using Lemma 3.5 with $2p+2$ for p we estimate the integrand

$$\int_{-a}^{a} |\partial^{\boldsymbol{n}}\tilde{g}(\mathbf{x})s(\mathbf{x})|\,\mathrm{d}x_1 \leqslant C(\boldsymbol{n}) \int_{-a}^{a} |\mathbf{x}|^{2p+1-|\boldsymbol{n}|}\,\mathrm{d}x_1 = C(\boldsymbol{n}) \int_{-a}^{a} |\mathbf{x}|^{2p-2m-1}\,\mathrm{d}x_1. \tag{3.16}$$

Since $x_2 \neq 0$ we can perform the change of variables $x_1 = x_2 s$ and $\mathrm{d}x_1 = x_2\,\mathrm{d}s$. We obtain

$$\int_{-a}^{a} |\mathbf{x}|^{2p-2m-1}\,\mathrm{d}x_1 = |x_2|^{2p-2m} \int_{-a/x_2}^{a/x_2} \sqrt{1+s^2}^{\,2p-2m-1}\,\mathrm{d}s$$
$$\leqslant |x_2|^{2p-2m} \int_{-\infty}^{\infty} \frac{1}{\sqrt{1+s^2}^{\,2m-2p+1}}\,\mathrm{d}s \leqslant C|x_2|^{2p-2m}, \tag{3.17}$$

since here $2m-2p+1 > 1$, which means that the integral is bounded.

Now we turn to the case $m = p$ and define the polynomial

$$Q(\mathbf{x}) = \sum_{|\ell|=2p+2} \frac{\partial^{\boldsymbol{\ell}}\tilde{g}(0)}{\partial \mathbf{x}^{\ell}} \frac{\mathbf{x}^{\boldsymbol{\ell}}}{\boldsymbol{\ell}!}.$$

Since $\partial^{\boldsymbol{k}} Q(0) = 0$ for $|\boldsymbol{k}| < 2p+2$, this polynomial has the property that

$$\partial^{\boldsymbol{k}}[\tilde{g}(\mathbf{x}) - Q(\mathbf{x})]|_{\mathbf{x}=0} = 0, \quad |\boldsymbol{k}| \leqslant 2p+2. \tag{3.18}$$

The function f can be split as

$$f(\mathbf{x}) = (\tilde{g}(\mathbf{x}) - Q(\mathbf{x}))s(\mathbf{x}) + Q(\mathbf{x})s(\mathbf{x}). \tag{3.19}$$

We can now use Lemma 3.5 for $(\tilde{g}-Q)s$ with $2p+2$ zero derivatives instead of only $2p+1$ as in the case $m>p$. This is allowed since $\tilde{g}$ has $2m+3=2p+3$ continuous derivatives. Then, in the same way as in (3.17) we find a constant C_1 such that

$$\int_{-a}^{a} |\partial^{\boldsymbol{n}}[\tilde{g}(\mathbf{x})-Q(\mathbf{x})]s(\mathbf{x})|\,\mathrm{d}x_1 \leqslant C_1|x_2|^{2p-2m}=C_1. \tag{3.20}$$

Next we seek to bound the $\boldsymbol{n}$th derivative of $Q(\mathbf{x})s(\mathbf{x})$ and proceed by splitting $\boldsymbol{n}=\tilde{\boldsymbol{n}}+\mathbf{e}_1$. We first take the $\tilde{\boldsymbol{n}}$th derivative and from Lemma 3.4 with $|\boldsymbol{k}|=2p+1$ and $|\boldsymbol{\alpha}|=2p+2$ we obtain

$$\partial^{\tilde{\boldsymbol{n}}}[Q(\mathbf{x})s(\mathbf{x})]=\sum_{|\ell|=2p+2}\frac{\partial^{\ell}\tilde{g}(0)}{\ell!\,\partial\mathbf{x}^{\ell}}P_{\tilde{\boldsymbol{n}},\ell}\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right)=:P\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right). \tag{3.21}$$

By further taking the derivative in the $\mathbf{e}_1$ direction and using the same differentiation as in Lemma 3.4 we have

$$\partial^{\boldsymbol{n}}[Q(\mathbf{x})s(\mathbf{x})]=\partial_{x_1}P\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right)=\frac{x_2}{|\mathbf{x}|^2}E\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right), \tag{3.22}$$

where E is another polynomial. We note that $\sup_x |E(\mathbf{x}/|\mathbf{x}|)|=:C_2<\infty$ as before. In order to bound the integral over $\partial^{\boldsymbol{n}}[Q(\mathbf{x})s(\mathbf{x})]$ we apply the change of variables $x_1=sx_2$ once more and obtain

$$\begin{aligned}\int_{-a}^{a}|\partial^{\boldsymbol{n}}[Q(\mathbf{x})s(\mathbf{x})]|\,\mathrm{d}x_1&=\int_{-a}^{a}\left|\frac{x_2}{|\mathbf{x}|^2}E\left(\frac{\mathbf{x}}{|\mathbf{x}|}\right)\right|\mathrm{d}x_1\leqslant C_2\int_{-a}^{a}\frac{|x_2|}{|\mathbf{x}|^2}\,\mathrm{d}x_1\\&=C_2\int_{-a/x_2}^{a/x_2}\frac{1}{1+s^2}\,\mathrm{d}x_1\leqslant C\int_{-\infty}^{\infty}\frac{1}{1+s^2}\,\mathrm{d}s=\pi C_2.\end{aligned} \tag{3.23}$$

Gathering (3.20) and (3.23) we finally have that for $p=m$,

$$\begin{aligned}\int_{-a}^{a}|\partial^{\boldsymbol{n}}(\tilde{g}(\mathbf{x})s(\mathbf{x}))|\,\mathrm{d}x_1&\leqslant\int_{-a}^{a}|\partial^{\boldsymbol{n}}[\tilde{g}(\mathbf{x})-Q(\mathbf{x})]s(\mathbf{x})|\,\mathrm{d}x_1+\int_{-a}^{a}|\partial^{\boldsymbol{n}}[Q(\mathbf{x})s(\mathbf{x})]|\,\mathrm{d}x_1\\&\leqslant C_1+\pi C_2,\end{aligned}$$

which concludes the proof of the lemma. □

We are now ready to prove Theorem 3.2. Let the compact support of f be denoted by D and suppose that $D\subset[-a,\ a]^2$. The error estimate will be obtained by evaluating two consequent approximations according to the split

$$\begin{aligned}\int_D f(\mathbf{x})\,\mathrm{d}\mathbf{x}-\mathcal{T}_h[f]&=\int_D f(\mathbf{x})\,\mathrm{d}\mathbf{x}-\int_{-a}^{a}T_h[f(\cdot,x_2)]\,\mathrm{d}x_2+\int_{-a}^{a}T_h[f(\cdot,x_2)]\,\mathrm{d}x_2-\mathcal{T}_h[f]\\&=\int_{-a}^{a}I_1(x_2)\,\mathrm{d}x_2+\sum_{j\in\mathbb{Z}}I_2(jh)h,\end{aligned} \tag{3.24}$$

with

$$
\begin{aligned}
I_1(x) &= \int_{-a}^{a} f(x_1, x)\,\mathrm{d}x_1 - T_h[f(\cdot, x)], \\
I_2(x) &= \int_{-a}^{a} f(x, x_2)\,\mathrm{d}x_2 - T_h[f(x, \cdot)].
\end{aligned} \tag{3.25}
$$

We note that by Lemma 3.5 with p set to $2p+2$ we have $\lim_{x\to 0} f(\mathbf{x}) = 0$ and f can therefore be defined by continuity at the origin. This implies that both $I_1(x)$ and $I_2(x)$ are continuous at $x = 0$.

Since $f(\mathbf{x})$ is smooth when $x_2 \neq 0$ we obtain from the Euler–Maclaurin expansion (1.3) that

$$
I_1(x_2) = \frac{h^{2m+2}}{(2m+2)!} \int_{-a}^{a} B_{2m+2}\left(\left\{\frac{x_1 + a}{h}\right\}\right) \partial_{x_1}^{2m+2} f(\mathbf{x})\,\mathrm{d}x_1,
$$

for any $m \leqslant q$ and $x_2 \neq 0$. Therefore, since $B_{2m+2}(\{x\})$ is bounded,

$$
|I_1(x_2)| \leqslant C_m h^{2m+2} \int_{-a}^{a} |\partial_{x_1}^{2m+2} f(\mathbf{x})|\,\mathrm{d}x_1,
$$

for $m \leqslant q$ and $x_2 \neq 0$. We distinguish two cases according to whether x_2 is in the vicinity of the origin where the singularity plays a bigger role or whether x_2 is away from the origin.

When $0 < |x_2| < h$ we take $m = p$ and obtain from Lemma 3.6 with $\boldsymbol{n} = (2p+2, 0)$ that

$$
|I_1(x_2)| \leqslant C_1 h^{2p+2}.
$$

When $|x_2| \geqslant h$ we take $m = q > p$ and obtain from Lemma 3.6 that

$$
|I_1(x_2)| \leqslant C_2 h^{2q+2} |x_2|^{2p-2q}.
$$

Now, since $I_1(x_2)$ is continuous at $x_2 = 0$ the integral can be bounded as

$$
\begin{aligned}
\int_{-a}^{a} |I_1(x_2)|\,\mathrm{d}x_2 &\leqslant C_1 h^{2p+2} \int_{-h}^{h} \mathrm{d}x_2 + C_2 h^{2q+2} \int_{a \geqslant |x_2| > h} |x_2|^{2p-2q}\,\mathrm{d}x_2 \\
&= 2C h^{2p+3} + 2C h^{2q+2} \frac{h^{2p-2q+1} - a^{2p-2q+1}}{2p-2q+1} < C h^{2p+3}.
\end{aligned} \tag{3.26}
$$

For $I_2(jh)$ we obtain, exactly as above,

$$
|I_2(jh)| \leqslant C h^{2q+2} |jh|^{2p-2q} = C h^{2p+2} |j|^{2p-2q}, \quad |j| > 1.
$$

For $j = 0$ we use the fact that I_2 is continuous at $x = 0$. The same estimate as above then gives

$$
|I_2(0)| = \lim_{x\to 0} |I_2(x)| \leqslant C h^{2p+2}.
$$

This leads to

$$
\sum_{j\in\mathbb{Z}} |I_2(jh)| h \leqslant |I_2(0)| h + \sum_{|j|\geqslant 1} |I_2(jh)| h \leqslant C h^{2p+3} + C h^{2p+3} \sum_{|j|\geqslant 1} j^{2p-2q} \leqslant C h^{2p+3}.
$$

Using this and (3.26) we get finally get, from (3.24),

$$\left|\int_D f(\mathbf{x})\,\mathrm{d}\mathbf{x} - \mathcal{T}_h[f]\right| \leqslant \int_{-a}^{a} |I_1(x_2)|\,\mathrm{d}x_2 + \sum_{j\in\mathbb{Z}} |I_2(jh)h| \leqslant Ch^{2p+3},$$

which concludes the proof of Theorem 3.2.

3.2 *Accuracy of the corrected trapezoidal rule*

The corrected trapezoidal rule consists of the punctured trapezoidal rule and a correction operator (2.15). The vector of correction weights $\bar{\boldsymbol{\omega}}$ is defined as the solution to system (2.13),

$$KI(h)\boldsymbol{\omega}(h) = \boldsymbol{c}(h),$$

as $h \to 0$. We assume throughout this text that the weights $\boldsymbol{\omega}(h)$ are well-defined solutions of this system for sufficiently small h. In two dimensions we also need to assume that the converged values $\bar{\boldsymbol{\omega}}$ obtained as the limit $\boldsymbol{\omega}(h) \to \bar{\boldsymbol{\omega}}$ when $h \to 0$ are well defined; in one dimension this follows from Lemma 3.8. Theorem 3.7 gives a proof of the convergence rate for the new quadrature rule in both one and two dimensions based on the assumption that the modified weights are bounded. When the nonconverged weights $\boldsymbol{\omega}(h)$ are used the convergence rate is $\mathcal{O}(h^{2p+2+\gamma+d})$. In the more practical case, when the converged weights $\bar{\boldsymbol{\omega}}$ are used, we prove that the convergence rate of the full rule depends on the convergence rate of the weights—if this rate is fast enough for some g then the overall convergence rate is unaffected. In one dimension we furthermore show that this fast rate can be obtained by choosing a flat enough g; see Lemma 3.8. Although we do not prove it, strong numerical evidence confirms that Lemma 3.8 and the overall rate $\mathcal{O}(h^{2p+2+\gamma+d})$ hold also in two dimensions.

THEOREM 3.7 Given a function $\phi \in C^{2q+2}(\mathbb{R}^d)$ compactly supported and a singular function

$$s(\mathbf{x}) = |\mathbf{x}|^{\gamma} \quad \text{with} \begin{cases} \gamma \in (-1,0), & \mathbf{x} \in \mathbb{R}, \\ \gamma = -1, & \mathbf{x} \in \mathbb{R}^2, \end{cases}$$

consider the modified quadrature applied to $f = \phi \cdot s$ written in operator form as

$$Q_h^p[\phi \cdot s] = T_h^0[\phi \cdot s] + A_h^p[\phi],$$

which corresponds to (2.14) with the correction operators (2.16) in one dimension and (2.15) in two dimensions. Let $g \in C_c^{2q+2}(\mathbb{R}^d)$ be a radially symmetric function such that $g(0) = 1$ and $\partial^{\boldsymbol{k}} g(0) = 0$ for $\boldsymbol{k} \leqslant 2p+1$ with $p < q$. Moreover, let $\boldsymbol{\omega}(h)$ be the solution of (2.13) for this g. Then the approximation error satisfies

$$|Q_h^p[\phi \cdot s] - I[\phi \cdot s]| \leqslant C(h^{2p+2+\gamma+d} + h^{\gamma+d}|\boldsymbol{\omega}(h) - \bar{\boldsymbol{\omega}}|), \tag{3.27}$$

where $I[\phi \cdot s]$ is the analytical integral. In one dimension, by using Lemma 3.8 the estimate leads to

$$|Q_h^p[\phi \cdot s] - I[\phi \cdot s]| \leqslant Ch^{2p+2+\gamma+d}. \tag{3.28}$$

Finally, if $\tilde{Q}_h^p$ is the quadrature rule where the nonconverged weights $\boldsymbol{\omega}(h)$ are used instead of $\bar{\boldsymbol{\omega}}$ in the correction operator, then

$$|\tilde{Q}_h^p[\phi \cdot s] - I[\phi \cdot s]| \leqslant Ch^{2p+2+\gamma+d}, \tag{3.29}$$

in both one and two dimensions.

Proof. We start by defining $P_\phi(\mathbf{x})$ as the Taylor polynomial of order $2p+1$ of ϕ at the origin,

$$P_\phi(\mathbf{x}) := \sum_{|\boldsymbol{\alpha}|=0}^{2p+1} \frac{\mathbf{x}^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!} \frac{\partial^{\boldsymbol{\alpha}} \phi(0)}{\partial \mathbf{x}^{\boldsymbol{\alpha}}}. \tag{3.30}$$

We furthermore define the compactly supported function $\tilde{\phi}(\mathbf{x}) = P_\phi(\mathbf{x})g(\mathbf{x})$ which is an approximation of $\phi(\mathbf{x})$ close to $\mathbf{x} = 0$. Indeed, for $|\boldsymbol{k}| < 2p+2$,

$$\partial^{\boldsymbol{k}} \tilde{\phi}(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{0}} = \sum_{\boldsymbol{\ell}+\boldsymbol{r}=\boldsymbol{k}} \frac{\boldsymbol{k}!}{\boldsymbol{r}!\boldsymbol{\ell}!} \partial^{\boldsymbol{\ell}} P_\phi(\mathbf{x}) \partial^{\boldsymbol{r}} g(\mathbf{x}) \Bigg|_{\mathbf{x}=\mathbf{0}} = \partial^{\boldsymbol{k}} P_\phi(\mathbf{x})\big|_{\mathbf{x}=\mathbf{0}} = \partial^{\boldsymbol{k}} \phi(\mathbf{0}),$$

and as a consequence,

$$\partial^{\boldsymbol{k}}[\phi(\mathbf{x}) - \tilde{\phi}(\mathbf{x})]|_{\mathbf{x}=\mathbf{0}} = 0, \quad |\boldsymbol{k}| < 2p+2. \tag{3.31}$$

In order to determine the order of convergence of $Q_h^p[f] - I[f]$ we split it as

$$\begin{aligned} Q_h^p[\phi \cdot s] - I[\phi \cdot s] &= T_h^0[\phi \cdot s] + A_h^p[\phi] - I[\phi \cdot s] \\ &= A_h^p[\phi - \tilde{\phi}] + (T_h^0 - I)[(\phi - \tilde{\phi}) \cdot s] + (Q_h^p - I)[\tilde{\phi} \cdot s] \\ &:= E_1 + E_2 + E_3, \end{aligned} \tag{3.32}$$

and treat these three terms separately.

To estimate E_1 we first note that (3.31) implies that, for all $\mathbf{x} \in \mathbb{R}^d$,

$$|\phi(\mathbf{x}) - \tilde{\phi}(\mathbf{x})| \leqslant C|\mathbf{x}|^{2p+2}, \quad C = \sup_{\substack{\mathbf{x}\in\mathbb{R}^d \\ |\boldsymbol{k}|=2p+2}} \frac{1}{\boldsymbol{k}!} |\partial^{\boldsymbol{k}}(\phi(\mathbf{x}) - \tilde{\phi}(\mathbf{x}))| < \infty.$$

Also using (2.5) and (2.15) we then get

$$\begin{aligned} |E_1| = |A_h^p[\phi - \tilde{\phi}]| &\leqslant Ca(h) \sup_{\boldsymbol{\beta}\in\mathcal{L}_p} [\phi(\boldsymbol{\beta}h) - \tilde{\phi}(\boldsymbol{\beta}h)] \leqslant Ch^{\gamma+d} \sup_{\boldsymbol{\beta}\in\mathcal{L}_p} |\boldsymbol{\beta}h|^{2p+2} \\ &\leqslant Ch^{2p+2+\gamma+d}, \end{aligned} \tag{3.33}$$

where we assumed that the weights $\bar{\boldsymbol{\omega}}$ are bounded.

To bound E_2 we use Theorem 3.2 in two dimensions and Theorem 3.1 in one dimension, yielding

$$|E_2| = |(T_h^0 - I)[\phi \cdot s - \tilde{\phi} \cdot s]| \leqslant Ch^{2p+2+\gamma+d}. \tag{3.34}$$

It remains to bound E_3. Using the fact that $\tilde{\phi}$ has the form $\tilde{\phi} = P_\phi g$ with P_ϕ defined in (3.30) we have

$$\begin{aligned} |E_3| = |Q_h^p[\tilde{\phi} \cdot s] - I[\tilde{\phi} \cdot s]| &\leqslant \sum_{|\boldsymbol{\alpha}|=0}^{2p+1} \frac{1}{\boldsymbol{\alpha}!} \left| \frac{\partial^{\boldsymbol{\alpha}} \phi(0)}{\partial \mathbf{x}^{\boldsymbol{\alpha}}} \right| |Q_h^p[g \cdot s \cdot \mathbf{x}^{\boldsymbol{\alpha}}] - I[g \cdot s \cdot \mathbf{x}^{\boldsymbol{\alpha}}]| \\ &\leqslant C \sum_{|\boldsymbol{\alpha}|=0}^{2p+1} |T_h^0[g \cdot s \cdot \mathbf{x}^{\boldsymbol{\alpha}}] - I[g \cdot s \cdot \mathbf{x}^{\boldsymbol{\alpha}}] + A_h^p[g \cdot \mathbf{x}^{\boldsymbol{\alpha}}]|. \end{aligned} \tag{3.35}$$

We now want to show that the terms inside the sum in (3.35) are zero if α_1 and/or α_2 in $\boldsymbol{\alpha} = (\alpha_1, \alpha_2)$ is odd. Since g is radially symmetric, $g(x_1, x_2) = g(\pm x_1, \pm x_2)$ for all combinations of signs. The same holds for s. Therefore,

$$\begin{aligned} I[g \cdot s \cdot \mathbf{x}^{\boldsymbol{\alpha}}] &= \int g(\mathbf{x}) s(\mathbf{x}) \mathbf{x}^{\boldsymbol{\alpha}} \, \mathrm{d}\mathbf{x} \\ &= \int_{x_1 \geqslant 0, x_2 \geqslant 0} g(\mathbf{x}) s(\mathbf{x}) [x_1^{\alpha_1} x_2^{\alpha_2} + (-x_1)^{\alpha_1} x_2^{\alpha_2} \\ &\quad + x_1^{\alpha_1} (-x_2)^{\alpha_2} + (-x_1)^{\alpha_1} (-x_2)^{\alpha_2}] \, \mathrm{d}\mathbf{x} \\ &= \int_{x_1 \geqslant 0, x_2 \geqslant 0} g(\mathbf{x}) s(\mathbf{x}) x_1^{\alpha_1} x_2^{\alpha_2} [1 + (-1)^{\alpha_1} + (-1)^{\alpha_2} + (-1)^{\alpha_1+\alpha_2}] \, \mathrm{d}\mathbf{x}, \end{aligned}$$

and this sum vanishes for α_1 and/or α_2 odd. In a similar way we obtain $T_h^0[g \cdot s \cdot \mathbf{x}^{\boldsymbol{\alpha}}] = 0$ for α_1 and/or α_2 odd. In one dimension the corresponding expressions are clearly zero if α is odd. For the operator A_h^p in (2.15) we have

$$\begin{aligned} A_h^p[g \cdot \mathbf{x}^{\boldsymbol{\alpha}}] &= a(h) \sum_{q=0}^{p} \sum_{m=0}^{[q/2]} \bar{\omega}_q^m \sum_{\boldsymbol{\beta} \in \mathcal{G}_q^m} g(\boldsymbol{\beta} h)(\boldsymbol{\beta} h)^{\boldsymbol{\alpha}} \\ &= a(h) \sum_{q=0}^{p} \sum_{m=0}^{[q/2]} C_q^m \bar{\omega}_q^m h^{\boldsymbol{\alpha}} \sum_{\boldsymbol{\beta} \in \mathcal{G}_q^m} \boldsymbol{\beta}^{\boldsymbol{\alpha}}. \end{aligned} \tag{3.36}$$

Here, we used the fact that $g(\boldsymbol{\beta} h)$ is constant for all $\boldsymbol{\beta} \in \mathcal{G}_q^m$ and we have called this constant C_q^m. Furthermore, let $\boldsymbol{\beta} = (\beta_1, \beta_2)$. Since $(\pm\beta_1, \pm\beta_2) \in \mathcal{G}_q^m$ if $\boldsymbol{\beta} \in \mathcal{G}_q^m$, then

$$\begin{aligned} \sum_{\boldsymbol{\beta} \in \mathcal{G}_q^m} \boldsymbol{\beta}^{\boldsymbol{\alpha}} &= \sum_{\boldsymbol{\beta} \in \mathcal{G}_q^m} \frac{\beta_1^{\alpha_1} \beta_2^{\alpha_2} + (-\beta_1)^{\alpha_1} \beta_2^{\alpha_2} + \beta_1^{\alpha_1} (-\beta_2)^{\alpha_2} + (-\beta_1)^{\alpha_1} (-\beta_2)^{\alpha_2}}{4} \\ &= \sum_{\boldsymbol{\beta} \in \mathcal{G}_q^m} \boldsymbol{\beta}^{\boldsymbol{\alpha}} \frac{1 + (-1)^{\alpha_1} + (-1)^{\alpha_2} + (-1)^{\alpha_1} (-1)^{\alpha_2}}{4} = 0, \end{aligned} \tag{3.37}$$

if α_1 or α_2 is odd. Hence, we have shown that the terms in (3.35) containing odd polynomials vanish. Retaining only the even polynomials, we write the sum as

$$|E_3| \leqslant C \sum_{|\boldsymbol{\alpha}|=0}^{p} |T_h^0[g \cdot s \cdot \mathbf{x}^{2\boldsymbol{\alpha}}] - I[g \cdot s \cdot \mathbf{x}^{2\boldsymbol{\alpha}}] + A_h^p[g \cdot \mathbf{x}^{2\boldsymbol{\alpha}}]|. \tag{3.38}$$

This sum is over all $\boldsymbol{\alpha} \in \mathcal{M}_p$ as defined in (2.11). By (2.12) the first difference in the sum may be rewritten

$$T_h^0[g \cdot s \cdot \mathbf{x}^{2\boldsymbol{\alpha}}] - I[g \cdot s \cdot \mathbf{x}^{2\boldsymbol{\alpha}}] = -a(h) \sum_{q=0}^{p} \sum_{m=0}^{[q/2]} \omega_q^m(h) \sum_{\boldsymbol{\beta} \in \mathcal{G}_q^m} g(\boldsymbol{\beta}h)(\boldsymbol{\beta}h)^{2\boldsymbol{\alpha}}.$$

From (3.38), using the formula above and also the definition of A_h^p in (2.15), we obtain

$$\begin{aligned} |E_3| &\leqslant C'a(h) \sum_{\boldsymbol{\alpha} \in \mathcal{M}_p} \sum_{q=0}^{p} \sum_{m=0}^{[q/2]} |\omega_q^m(h) - \bar{\omega}_q^m||g(\boldsymbol{\beta}h)||(\boldsymbol{\beta}h)|^{2|\boldsymbol{\alpha}|} \\ &\leqslant Ch^{\gamma+d}|\boldsymbol{\omega}(h) - \bar{\boldsymbol{\omega}}|. \end{aligned}$$

By also using (3.33), (3.34) and the split (3.32), the result in (3.27) follows. Finally, to prove (3.29) we just note that if the weights are changed, the estimate (3.33) for E_1 can be done in precisely the same way, while clearly $E_3 = 0$. □

The estimate (3.28) of the theorem is a consequence of the following Lemma 3.8, upon noting that we can always find a function $g(x)$ satisfying the assumptions of the theorem with $q \geqslant 2p + (1+\gamma)/2$. Then $\mathcal{O}(h^{2q+1-\gamma-2p}) \leqslant \mathcal{O}(h^{2p+2})$ and (3.39) inserted in (3.27) gives (3.28).

LEMMA 3.8 Let p and q be integers such that $0 \leqslant p < q$ and $2q+1 > \gamma + 2p$. Suppose $g(x) \in C_c^{2q+2}(\mathbb{R})$ is an even function with g as in Theorem 3.7. Then the approximate weights $\boldsymbol{\omega}(h)$ given as the solution of (2.13) for this g converge to $\bar{\boldsymbol{\omega}}$ and satisfy the error estimate

$$|\boldsymbol{\omega}(h) - \bar{\boldsymbol{\omega}}| \leqslant C(h^{2p+2} + h^{2q+1-\gamma-2p}). \tag{3.39}$$

Proof. We claim that $\bar{\boldsymbol{\omega}}$ is given as a solution to

$$K\bar{\boldsymbol{\omega}} = \bar{\boldsymbol{c}}(\gamma),$$

where $\bar{\boldsymbol{c}}(\gamma)$ is defined as $\bar{\boldsymbol{c}} = (\bar{c}_0, \ldots, \bar{c}_{N_p-1})$ with $\bar{c}_i = \bar{c}(\gamma + 2i)$ and $\bar{c}(\gamma)$ given in Theorem 3.1. Note that since K is a Vandermonde matrix with $K_{ij} = 2j^{2i}$ it is nonsingular, so $\bar{\boldsymbol{\omega}}$ is well defined. Furthermore with the notation in Section 2.2 and by Theorem 3.1,

$$\begin{aligned} h^{\gamma+1+2i} c_i(h) &= \int g(x)s(x)x^{2i}\,\mathrm{d}x - T_h^0[g \cdot s \cdot x^{2i}] \\ &= g(0)h^{\gamma+1+2i}\bar{c}_i + \mathcal{O}(h^{2p+\gamma+3+2i} + h^{2q+2}). \end{aligned} \tag{3.40}$$

Therefore,

$$|c_i(h) - \bar{c}_i| \leqslant C(h^{2p+2} + h^{2q+2-\gamma-1-2i}) \leqslant C'(h^{2p+2} + h^{2q+1-\gamma-2p}). \tag{3.41}$$

By Taylor expanding $\tilde{I}(h)$ around the origin and using the fact that $g(x)$ has $2p+1$ vanishing derivatives at the origin, we also have

$$|\tilde{I}(h) - I| \leqslant Ch^{2p+2}, \tag{3.42}$$

with I the identity matrix. The result (3.39) now follows since

$$\begin{aligned} |\boldsymbol{\omega}(h) - \bar{\boldsymbol{\omega}}| &= |\tilde{I}(h)^{-1}K^{-1}\boldsymbol{c}(h) - K^{-1}\bar{\boldsymbol{c}}(\gamma)| \\ &= |K^{-1}(\boldsymbol{c}(h) - \bar{\boldsymbol{c}}(\gamma)) + (\tilde{I}(h)^{-1} - I)K^{-1}\boldsymbol{c}(h)| \\ &\leqslant C|\boldsymbol{c}(h) - \bar{\boldsymbol{c}}(\gamma)| + C'|\tilde{I}(h) - I|. \end{aligned} \tag{3.43}$$

Using (3.41) and (3.42), this proves the lemma. □

4. Numerical results

The correction weights for the quadrature rules depend on the singularity and must be computed and tabulated for each singularity under consideration. In this section we first discuss the computation of the weights, and then provide tabulated weights and discuss examples in one and two dimensions.

4.1 *Computing the correction weights*

The vector of correction weights $\boldsymbol{\omega}(h)$ can be obtained as solutions to system (2.13) with the aid of a smooth and compactly supported function. How fast these weights converge to their limiting values $\bar{\boldsymbol{\omega}}$ depends on the number of vanishing derivatives that the compactly supported function has at the origin—see Lemma 3.8. In practice, we do not choose a compactly supported function but $g(x) = e^{-|x|^{2k}}$ in such way that it is properly decayed at the boundaries of the domain. Note that for increasing values of k this function has an increasing number of derivatives that vanish at the origin.

In one dimension the vector of converged weights $\bar{\boldsymbol{\omega}}$ can be obtained as the solution of (A.2), using the closed form expression of $\bar{c}(\gamma)$, and we use these to measure the errors in $\boldsymbol{\omega}(h)$. In Fig. 2 the convergence rate of the weights is displayed for $g(x) = e^{-x^2}$ and $g(x) = e^{-x^4}$. In the first case, only the first derivative vanishes at the origin and therefore by Lemma 3.8 we expect a convergence order $\mathcal{O}(h^2)$. Similarly, for e^{-x^4} all the derivatives up to third-order evaluate to zero at the origin and thus we expect $\mathcal{O}(h^4)$ convergence. The numerical tests confirm the expected orders of convergence.

In two dimensions, we do not have a direct way to obtain the converged weights and system (2.13) has to be solved as $h \to 0$. A bottleneck in this procedure is the ill conditioning of the linear system; as the number of modified weights increases the reciprocal condition number of the system reaches epsilon of the machine. The aim is to obtain the value of the weights with double precision. Therefore, the systems are solved in multiple precision arithmetic through straightforward Gaussian elimination followed by repeated Richardson extrapolation.

For $g(\mathbf{x}) = e^{-|\mathbf{x}|^{2k}}$ the order of convergence of the weights is $\mathcal{O}(h^{2k})$ and a larger value of k can be used to speed up the convergence. In Fig. 3, for system (2.13) with $p = 3$, we show how the choice of k controls the convergence of the weights with respect to the condition number of the system, $\kappa(A)$. Note that the condition number depends only weakly on the choice of g for a fixed h (the data points corresponding to the same h essentially line up along vertical lines). On the horizontal axis we can follow the growth of the condition number $\kappa(A)$, while on the vertical axis we can read the error in approximating the weights. To achieve an error $\|\bar{\boldsymbol{\omega}} - \boldsymbol{\omega}(h)\|_\infty$ below a prescribed tolerance, the condition number will be lower for a larger k, and fewer digits will be lost in the calculations. Hence, not as many digits are

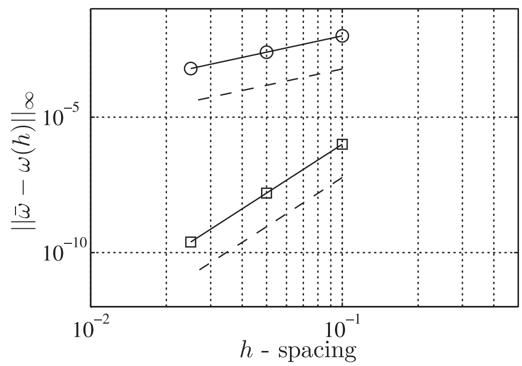

FIG. 2. Error of the weights estimation: circles represent e^{-x^2}; boxes represent e^{-x^4}; dashed lines represent the slopes of the expected order of convergence: $\mathcal{O}(h^2)$; $\mathcal{O}(h^4)$.

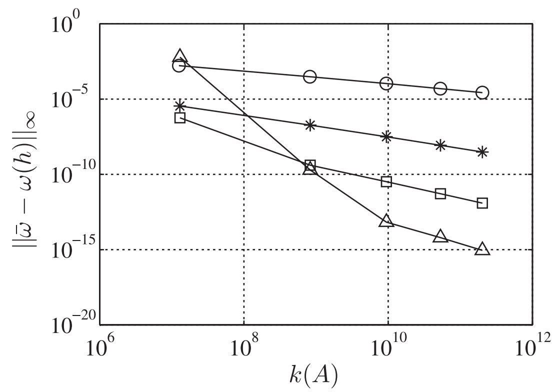

FIG. 3. Error in estimating the weights $\|\bar{\boldsymbol{\omega}} - \boldsymbol{\omega}(h)\|_\infty$ versus the condition number of the system $\kappa(A)$ ($p = 3$, two-dimensional): circles represent $e^{-|\mathbf{x}|^2}$; asterisks represent $e^{-|\mathbf{x}|^4}$; squares represent $e^{-|\mathbf{x}|^6}$; triangles represent $e^{-|\mathbf{x}|^8}$.

needed in the multiprecision arithmetic, and the system can be solved much faster. However, it can also be seen from Fig. 3 that once we use $e^{-|\mathbf{x}|^8}$, the computations for large h display a worse error than for lower exponents of the Gaussian. This is due to the difficulty in numerically resolving the Gaussian once the exponent of $e^{-|\mathbf{x}|^{2k}}$ increases. This implies that it will not be feasible to increase k indefinitely and we must settle for some intermediate value. Consequently, in practice we shall set up system (2.13) for the function $e^{-|\mathbf{x}|^6}$, compute several solutions $\boldsymbol{\omega}(h)$ and use Richardson extrapolation as a final step in retrieving $\bar{\boldsymbol{\omega}}$ as given in Table 2.

4.2 *Applying the quadrature rules*: *a one-dimensional example*

In this section, we study the convergence rates of the newly developed quadrature rules when applied to a singularity of type $|x|^\gamma$. We use (2.14) and (2.16) with correction weights at $2p+1$ points, obtained by solving system (A.2). We consider two cases.

In the first case, we take $f(x) = \cos(x)|x|^\gamma$ with $\gamma = -0.8$ and $p = 2$. We include boundaries, but use high-order boundary corrections given in Alpert (1995) so that the boundaries yield lower errors than the

TABLE 2 *Modified weights for the* $1/|\mathbf{x}|$ *singularity in two dimensions*

q	$\mathcal{O}(h^{2q+3})$	Discretization points	Modified weights
0	3	$\mathcal{G}_0^0 = \{(0,0)\}$	$\bar{\omega}_0^0 = 3.9002649200019564 \times 10^0$
1	5	$\mathcal{G}_0^0 = \{(0,0)\}$	$\bar{\omega}_0^0 = 3.6714406096247369 \times 10^0$
		$\mathcal{G}_1^0 = \{(\pm1,0),(0,\pm1)\}$	$\bar{\omega}_1^0 = 5.7206077594304738 \times 10^{-2}$
2	7	$\mathcal{G}_0^0 = \{(0,0)\}$	$\bar{\omega}_0^0 = 3.6192550095006482 \times 10^0$
		$\mathcal{G}_1^0 = \{(\pm1,0),(0,\pm1)\}$	$\bar{\omega}_1^0 = 7.0478261675350094 \times 10^{-2}$
		$\mathcal{G}_2^1 = \{(\pm1,\pm1)\}$	$\bar{\omega}_2^1 = 6.1845239404762928 \times 10^{-3}$
		$\mathcal{G}_2^0 = \{(\pm2,0),(0,\pm2)\}$	$\bar{\omega}_2^0 = -6.4103079904994854 \times 10^{-3}$
3	9	$\mathcal{G}_0^0 = \{(0,0)\}$	$\bar{\omega}_0^0 = 3.5956326153661837 \times 10^0$
		$\mathcal{G}_1^0 = \{(\pm1,0),(0,\pm1)\}$	$\bar{\omega}_1^0 = 7.6498210003072550 \times 10^{-2}$
		$\mathcal{G}_2^1 = \{(\pm1,\pm1)\}$	$\bar{\omega}_2^1 = 1.0726043096799093 \times 10^{-2}$
		$\mathcal{G}_2^0 = \{(\pm2,0),(0,\pm2)\}$	$\bar{\omega}_2^0 = -1.0861970941933728 \times 10^{-2}$
		$\mathcal{G}_3^1 = \{(\pm2,\pm1),(\pm1,\pm2)\}$	$\bar{\omega}_3^1 = -5.6768989454035010 \times 10^{-4}$
		$\mathcal{G}_3^0 = \{(\pm3,0),(0,\pm3)\}$	$\bar{\omega}_3^0 = 9.3117379008582382 \times 10^{-4}$
4	11	$\mathcal{G}_0^0 = \{(0,0)\}$	$\bar{\omega}_0^0 = 3.5816901196890991 \times 10^0$
		$\mathcal{G}_1^0 = \{(\pm1,0),(0,\pm1)\}$	$\bar{\omega}_1^0 = 8.0270822919205118 \times 10^{-2}$
		$\mathcal{G}_2^1 = \{(\pm1,\pm1)\}$	$\bar{\omega}_2^1 = 1.3733352021301174 \times 10^{-2}$
		$\mathcal{G}_2^0 = \{(\pm2,0),(0,\pm2)\}$	$\bar{\omega}_2^0 = -1.4045613458587681 \times 10^{-2}$
		$\mathcal{G}_3^1 = \{(\pm2,\pm1),(\pm1,\pm2)\}$	$\bar{\omega}_3^1 = -1.1741498011806794 \times 10^{-3}$
		$\mathcal{G}_3^0 = \{(\pm3,0),(0,\pm3)\}$	$\bar{\omega}_3^0 = 1.9899412695107586 \times 10^{-3}$
		$\mathcal{G}_4^2 = \{(\pm2,\pm2)\}$	$\bar{\omega}_4^2 = 6.2476521748914537 \times 10^{-6}$
		$\mathcal{G}_4^1 = \{(\pm3,\pm1),(\pm1,\pm3)\}$	$\bar{\omega}_4^1 = 9.6911549656793913 \times 10^{-5}$
		$\mathcal{G}_4^0 = \{(\pm4,\pm0),(0,\pm4)\}$	$\bar{\omega}_4^0 = -1.5657382234231533 \times 10^{-4}$
5	13	$\mathcal{G}_0^0 = \{(0,0)\}$	$\bar{\omega}_0^0 = 3.5724020676062076 \times 10^0$
		$\mathcal{G}_1^0 = \{(\pm1,0),(0,\pm1)\}$	$\bar{\omega}_1^0 = 8.2931084474334645 \times 10^{-2}$
		$\mathcal{G}_2^1 = \{(\pm1,\pm1)\}$	$\bar{\omega}_2^1 = 1.5807226557430198 \times 10^{-2}$
		$\mathcal{G}_2^0 = \{(\pm2,0),(0,\pm2)\}$	$\bar{\omega}_2^0 = -1.6446295482375981 \times 10^{-2}$
		$\mathcal{G}_3^1 = \{(\pm2,\pm1),(\pm1,\pm2)\}$	$\bar{\omega}_3^1 = -1.6998553930113205 \times 10^{-3}$
		$\mathcal{G}_3^0 = \{(\pm3,0),(0,\pm3)\}$	$\bar{\omega}_3^0 = 2.9905345964354009 \times 10^{-3}$
		$\mathcal{G}_4^2 = \{(\pm2,\pm2)\}$	$\bar{\omega}_4^2 = 1.5896929239405025 \times 10^{-5}$
		$\mathcal{G}_4^1 = \{(\pm3,\pm1),(\pm1,\pm3)\}$	$\bar{\omega}_4^1 = 2.4136953002238568 \times 10^{-4}$
		$\mathcal{G}_4^0 = \{(\pm4,\pm0),(0,\pm4)\}$	$\bar{\omega}_4^0 = -4.0746367252001358 \times 10^{-4}$
		$\mathcal{G}_5^2 = \{(\pm3,\pm2),(\pm2,\pm3)\}$	$\bar{\omega}_5^2 = -8.0410642204279767 \times 10^{-7}$
		$\mathcal{G}_5^1 = \{(\pm4,\pm1),(\pm1,\pm4)\}$	$\bar{\omega}_5^1 = -1.7655194334677572 \times 10^{-5}$
		$\mathcal{G}_5^0 = \{(\pm5,\pm0),(0,\pm5)\}$	$\bar{\omega}_5^0 = 2.8620023884705339 \times 10^{-5}$

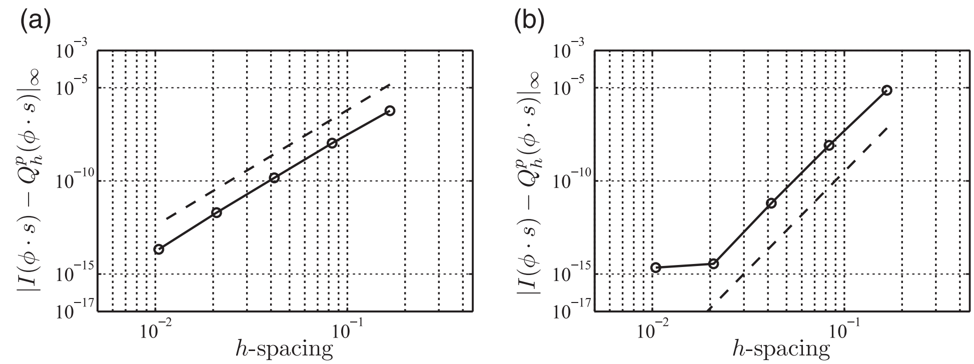

FIG. 4. Convergence tests for various singularities: circles represent computed accuracy; the dashed line represents the slope of the theoretical order of convergence. (a) $p = 2$, $\gamma = -0.8$; $\mathcal{O}(h^{8.2})$; boundary corrections are used; (b) $p = 4$, $\gamma = -0.5$; $\mathcal{O}(h^{10.5})$; compactly supported integrand.

TABLE 3 *Weights for the quadrature rule* Q_h^p, *with* $p = 4$ *for* $s(x) = |x|^{-0.5}$

Discretization points	Weights
$j = 0$	$\omega_0 = 2.8436476480899424$
$j = \pm 1$	$\omega_1 = 4.4010623268195800 \times 10^{-2}$
$j = \pm 2$	$\omega_2 = -6.2404540776693907 \times 10^{-3}$
$j = \pm 3$	$\omega_3 = 8.1883632187304387 \times 10^{-4}$
$j = \pm 4$	$\omega_4 = -5.8320747783912244 \times 10^{-4}$

singularity. The expected convergence rate is $\mathcal{O}(h^{2p+3+\gamma}) = \mathcal{O}(h^{6.2})$ and to preserve this accuracy we use boundary corrections of order $\mathcal{O}(h^8)$. The result agrees well with the theory, as reported in Fig. 4(a).

In the second case, we take $f(x) = \exp^{-x^2} \cos(x)|x|^\gamma$ with $\gamma = -0.5$ and $p = 4$. In this case the function is essentially zero on the boundaries and no boundary correction is needed. Theory predicts a convergence rate of $\mathcal{O}(h^{10.5})$ which holds up well; see Fig. 4(b). We also record in Table 3 the correction weights for the quadrature rule used in this case ($p = 4$ and $\gamma = -0.5$).

4.3 *Applying the quadrature rules*: *a two-dimensional example*

Consider an essentially compactly supported function, e.g., $\phi(x, y) = \cos(x)\, e^{-(x^2+y^2)}$ and evaluate

$$\int_{-8}^{8} \int_{-8}^{8} \frac{\phi(x, y)}{\sqrt{x^2 + y^2}} \,\mathrm{d}x\,\mathrm{d}y. \tag{4.1}$$

On this chosen integral we test the set of quadrature rules Q_h^p, with $p = 0, \ldots, 5$, as defined in (2.14). The improvement in accuracy as p increases can be observed in Fig. 5 and in Table 4 where the order of convergence obtained through numerical experiment is compared with the theoretical one. The expected order of convergence for Q_h^p is 13. In practice even higher-order quadrature rules ($p > 5$) do not seem to result in better accuracy; in the asymptotic range, round-off errors dominate in double precision.

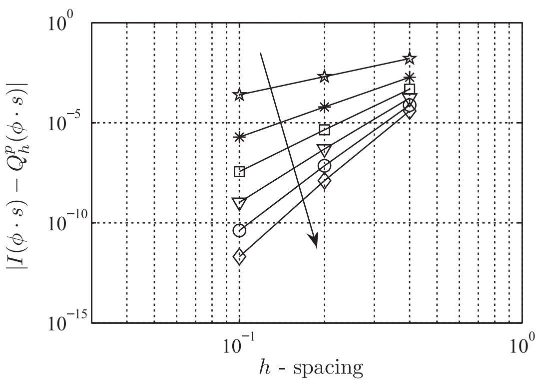

FIG. 5. Accuracy results for increasing values of p (in direction of arrow): stars represent $p = 0$; asterisks represent $p = 1$; squares represent $p = 2$; triangles represent $p = 3$; circles represent $p = 4$; diamonds represent $p = 5$.

TABLE 4 *Computed order of convergence, numerical versus theoretical—two-dimensional case*

	Convergence order	
p	Theoretical	Numerical
0	3	3.0040
1	5	4.9854
2	7	6.9356
3	9	8.8563
4	11	10.7476
5	13	12.6107

5. Conclusion

We have constructed and also proved the accuracy of high-order quadrature rules that handle singular functions of the type $s(x) = |x|^\gamma$ with $\gamma > -1$ in one dimension and $\gamma = -1$ in two dimensions. The quadrature rules are based on the well-known trapezoidal rule, but with modified weights close to the singularity. They can be applied in a straightforward manner by using the modified weights which have been computed and tabulated in this paper.

In the construction of the quadrature rules we used compactly supported functions to annihilate boundary errors and accelerate the convergence of the correction weights. If the quadrature rule is to be applied to functions that are neither periodic nor compactly supported within the domain, it should be combined with boundary corrections for the trapezoidal rule of sufficiently high order to exhibit the full convergence order it has been designed to have. The correction operator associated with the singularity remains the same whether or not boundary corrections are necessary.

The modified weights are obtained as the solution of an ill-conditioned linear system of equations. We have described how this system is set up and discussed its ill conditioning. The convergence rate of the weights depends on the *flatness* of the compactly supported function used to annihilate boundary errors, i.e., on the number of derivatives that vanish at the singular point. We illustrate this property in numerical examples and prove mathematically its validity in the one-dimensional case. With an improved convergence rate for the weights, a larger h can be used, which to some extent alleviates the ill-conditioning problem. To be able to compute the weights with 16 correct digits, a multiprecision library is used. In one dimension, we were able to find an analytical expression for the right-hand side of the system such that converged weights can be computed directly (see the Appendix).

The methodology for setting up the system for the weights can be extended also to other singularities, e.g., the fundamental solution of the Stokes equations (see Marin *et al.*, 2012) which is not radially symmetric in all its tensorial components as the functions $|x|^\gamma$, and more complicated symmetries, must be taken into account.

The integration of $1/|\mathbf{x}|$ in $\mathbb{R}^2$ as considered here, can also be viewed as an integration of the fundamental solution of the Laplace equation over a flat surface in $\mathbb{R}^3$. This relates to the discretization of boundary integral formulations, where integrals are to be evaluated over the boundaries of the domain, be it an outer boundary, the surface of a scattering object in an electromagnetic application or the surface of an immersed particle in Stokes flow. We therefore plan to extend this work to also consider the integration of weakly singular integrals over more general smooth surfaces.

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Appendix. Analytical expression for weights (one-dimensional case)

For the one-dimensional case we are able to provide an analytical expression for the weights. The weights are a solution, as a function of h, of system (2.13) which reads

$$K\tilde{I}(h)\boldsymbol{\omega}(h) = \boldsymbol{c}(h). \tag{A.1}$$

From Lemma 3.8 we know that $\tilde{I}(h)$ converges to the identity matrix and if we could obtain an analytical expression, $\bar{\boldsymbol{c}}(\gamma)$ which is the limit value of the right-hand side, the weights could be computed simply by solving a system independent of the discretization such as

$$K\bar{\boldsymbol{\omega}} = \bar{\boldsymbol{c}}(\gamma), \tag{A.2}$$

where the vector $\bar{\boldsymbol{c}}(\gamma)$ has elements $(\bar{c}_0, \ldots, \bar{c}_{N_p-1})$ with $\bar{c}_i = \bar{c}(\gamma + 2i)$. The function $\bar{c}(\gamma)$ was first encountered in Theorem 3.1 and consequently shown to have the form[1]

$$\bar{c}(\gamma) = \int_{-1}^{1} s(x)(1 - \psi(x))\,\mathrm{d}x - 4\Re \sum_{k=1}^{\infty} \frac{W(2\pi k)}{(2\pi k)^{2q}}.$$

In Lemma A2 we will show that $\bar{c}(\gamma) = -2\zeta(-\gamma)$, where ζ is the Riemann zeta function. In the proof we will make use of the expansion of $\zeta(\gamma)$ around the pole at $\gamma = 1$.

THEOREM A1 (Riemann zeta function) For all integers $q \geqslant 1$ and complex values γ with $\Re\gamma < 2q$,

$$\zeta(-\gamma) = -\frac{1}{\gamma+1} + \frac{1}{2} - \sum_{j=1}^{q} \frac{B_{2j}}{(2j)!} s^{(2j-1)}(1) - \frac{1}{(2q)!} \int_{1}^{\infty} s^{(2q)}(x) B_{2q}(\{x\})\,\mathrm{d}x,$$

where $s(x) = x^{\gamma}$.

[1] We use q instead of $q+1$ here for notational simplicity.

The result in Theorem A1 can be found, for instance, in Abramowitz & Stegun (1964, Formula 23.2.3, p. 807).

LEMMA A2 The expression of $\bar{c}(\gamma)$ corresponding to a singularity $s(x)=|x|^{\gamma}$ which generates the right-hand side to system (A.2) has the closed form expression

$$\bar{c}(\gamma)=-2\zeta(-\gamma),$$

where ζ is the Riemann zeta function.

Using definition (3.11) of $W(k)$ we have

$$\begin{aligned}
4\Re\sum_{k=1}^{\infty}\frac{W(2\pi k)}{(2\pi k)^{2q}} &= 4\Re\sum_{k=1}^{\infty}(2\pi \mathrm{i}k)^{-2q}\int_0^{\infty}\left(\frac{\mathrm{d}^{2q}}{\mathrm{d}x^{2q}}\psi(x)s(x)\right)e^{2\pi \mathrm{i}kx}\,\mathrm{d}x\\
&= 2\Re\sum_{k=1}^{\infty}(2\pi \mathrm{i}k)^{-2q}\int\left(\frac{\mathrm{d}^{q}}{\mathrm{d}x^{2q}}\psi(x)s(x)\right)e^{2\pi \mathrm{i}kx}\,\mathrm{d}x\\
&= \int\left(\frac{\mathrm{d}^{2q}}{\mathrm{d}x^{2q}}\psi(x)s(x)\right)\sum_{k\neq 0}\frac{e^{2\pi \mathrm{i}kx}}{(2\pi \mathrm{i}k)^{2q}}\,\mathrm{d}x\\
&= -\frac{1}{(2q)!}\int\left(\frac{\mathrm{d}^{2q}}{\mathrm{d}x^{2q}}\psi(x)s(x)\right)B_{2q}(\{x\})\,\mathrm{d}x,
\end{aligned}$$

where we used the formula for the Fourier series of $B_q(x)$, $0\leqslant x<1$. Thus,

$$\bar{c}(\gamma)=\int_{-1}^{1}s(x)(1-\psi(x))\,\mathrm{d}x+\frac{1}{(2q)!}\int\left(\frac{\mathrm{d}^{2q}}{\mathrm{d}x^{2q}}\psi(x)s(x)\right)B_{2q}(\{x\})\,\mathrm{d}x.$$

Since $B_{2q}(1-x)=B_{2q}(x)$ then by the symmetry of all functions,

$$\frac{1}{2}\bar{c}(\gamma)=\int_{0}^{1}s(x)(1-\psi(x))\,\mathrm{d}x+\frac{1}{(2q)!}\int_0^{\infty}\left(\frac{\mathrm{d}^{2q}}{\mathrm{d}x^{2q}}\psi(x)s(x)\right)B_{2q}(\{x\})\,\mathrm{d}x. \tag{A.3}$$

To evaluate the last integral in (A.3), we will now use the Euler–Maclaurin (Theorem 1.1) summation formula for the integral over $[0,1]$ and Theorem A1 for the rest. We also need the fact that since $\psi(x)\equiv 1$ for $x\geqslant 1$,

$$\left.\frac{\mathrm{d}^j}{\mathrm{d}x^j}\psi(x)s(x)\right|_{x=1}=s^{(j)}(1),\quad j\geqslant 0.$$

We get

$$\begin{aligned}
\frac{1}{(2q)!}\int_0^{\infty}\left(\frac{\mathrm{d}^{2q}}{\mathrm{d}x^{2q}}\psi(x)s(x)\right)B_{2q}(\{x\})\,\mathrm{d}x &= \frac{1}{(2q)!}\int_0^{1}\left(\frac{\mathrm{d}^{2q}}{\mathrm{d}x^{2q}}\psi(x)s(x)\right)B_{2q}(\{x\})\,\mathrm{d}x \\
&\quad + \frac{1}{(2q)!}\int_1^{\infty} s^{(2q)}(x)B_{2q}(\{x\})\,\mathrm{d}x \\
&= \int_0^1 \psi(x)s(x)\,\mathrm{d}x - \frac{1}{2}s(1) + \sum_{j=1}^{q}\frac{B_{2j}}{(2j)!}s^{(2j-1)}(1) \\
&\quad - \zeta(-\gamma) - \frac{1}{\gamma+1} + \frac{1}{2} - \sum_{j=1}^{q}\frac{B_{2j}}{(2j)!}s^{(2j-1)}(1) \\
&= \int_0^1 \psi(x)s(x)\,\mathrm{d}x - \zeta(-\gamma) - \int_0^1 s(x)\,\mathrm{d}x.
\end{aligned}$$

Together with (A.3), this shows that

$$\bar{c}(\gamma) = -2\zeta(-\gamma). \tag{A.4}$$