From high oscillation to rapid approximation III: Multivariate expansions

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Abstract

In this paper we expand upon the theme of modified Fourier expansions and extend the theory to a multivariate setting and to expansions in eigenfunctions of the Laplace–Neumann operator. We pay detailed attention to expansions in a d-dimensional cube and to an effective derivation of expansion coefficients there by means of quadratures of highly oscillatory integrals. Thus, we present asymptotic and Filon-type formulæ for an effective derivation of expansion coefficients and discuss their design and relative advantages. Such methods are effective only for large indices, hence we introduce and analyse alternative quadrature schemes that require relatively modest number of additional function evaluations.

1 Introduction

In this paper we revisit a theme that concerned us in two recent papers (Iserles & Nørsett 2006*a*, Iserles & Nørsett 2006*b*), namely rapidly-convergent expansion of smooth functions.

The point of departure in (Iserles & Nørsett 2006*a*) was the *modified Fourier basis*

$$\mathcal{H}_1 = \{\cos \pi n x \,:\, n \geq 0\} \cup \{\sin \pi(n - \tfrac{1}{2})x \,:\, n \geq 1\}.$$

Given a smooth f in $[-1, 1]$, which need not be periodic, we expand it in the form

$$\hat{f}_0^C + \sum_{n=1}^{\infty} [\hat{f}_n^C \cos \pi n x + \hat{f}_n^S \sin \pi(n - \tfrac{1}{2})x], \qquad (1.1)$$

where

$$\hat{f}_n^C = \int_{-1}^{1} f(x)\cos \pi n x \mathrm{d}x, \qquad \hat{f}_n^S = \int_{-1}^{1} f(x)\sin(n-\tfrac{1}{2})x \mathrm{d}x.$$

The main immediate advantage of (1.1), in comparison with the familiar Fourier expansion, is that the coefficients $\hat{f}_n^C$ and $\hat{f}_n^S$ exhibit $\mathcal{O}(n^{-2})$ decay for $n \gg 1$. This need be compared to the $\mathcal{O}(n^{-1})$ decay of conventional Fourier coefficients for *non-periodic* smooth functions and has two important consequences, one theoretical and the other computational. Firstly, for analytic f the expansion (1.1) converges uniformly to f in $[-1, 1]$. (We refer the reader to (Iserles & Nørsett 2006*a*) for considerably more detailed discussion of this issue, in particular to the question of convergence of functions that exhibit weaker smoothness.) Secondly, the more rapid decay of coefficients allows for the implementation of a range of highly effective modern quadrature methods for rapidly oscillating integrals (Huybrechs & Vandewalle 2006, Iserles & Nørsett 2005, Olver 2006*b*) in their computation. This means that for any prescribed accuracy we can evaluate $\hat{f}_n^C$ and $\hat{f}_n^S$ for $n \le m$ in just $\mathcal{O}(m)$ operations – computational cost that compares advantageously with the $m \log_2 m$ cost of FFT.

The underlying reason for the more rapid decay of expansion coefficients of modified Fourier has been identified in (Iserles & Nørsett 2006*b*): the functions in the basis $\mathcal{H}_1$ are all eigenfunctions of $\mathrm{d}^2/\mathrm{d}x^2$ and they obey zero Neumann boundary conditions at ± 1. (This should be compared with $\sin \pi n x$ from the conventional Fourier basis: also an eigenfunction of $\mathrm{d}^2/\mathrm{d}x^2$, but one that obeys zero Dirichlet boundary conditions at ± 1.) Zero boundary conditions annihilate the leading term in the asymptotic expansion of expansion coefficients in inverse powers of n, thereby leading to $\mathcal{O}(n^{-2})$ decay.

An immediate consequence of this identification of more rapid decay with zero Neumann boundary conditions is the construction of expansions that converge more rapidly than the modified Fourier expansion. Specifically, the coefficients of expansion

$$\sum_{n=0}^{\infty} \hat{f}_n u_n(x)$$

of a smooth function f in the eigenfunctions u_n of $\mathrm{d}^{2s}/\mathrm{d}x^{2s}$ for some $s \in \mathbb{N}$, equipped with the high-order Neumann boundary conditions

$$u_n^{(i)}(-1) = u_n^{(i)}(1) = 0, \qquad i = s, s+1, \ldots, 2s-1,$$

exhibit $\mathcal{O}(n^{-s-1})$ decay for $n \gg 1$ (Iserles & Nørsett 2006*b*).

The identification of rapid decay with zero Neumann boundary conditions allows an alternative generalisation with arguably even greater significance. Thus, suppose that $\Omega \in \mathbb{R}^d$ is a bounded, simply-connected domain with sufficiently smooth boundary. Let u_n be the nth eigenfunction of the Laplace operator $-\Delta$ in Ω, equipped with zero Neumann boundary conditions along $\partial\Omega$, and let λ_n be the corresponding eigenvalue, $n \ge 0$. Given a sufficiently smooth function f, defined on the closure of Ω, we consider the expansion

$$\sum_{n=0}^{\infty} \hat{f}_n u_n(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega, \tag{1.2}$$

where

$$\hat{f}_n = \int_{\Omega} f(\boldsymbol{\xi}) u_n(\boldsymbol{\xi}) \mathrm{d}V, \qquad n \ge 0. \tag{1.3}$$

We note from general theory of partial differential equations that, without loss of generality, $\lambda_0 = 0$, $\lambda_n > 0$ for $n \in \mathbb{N}$ and, provided that we arrange eigenvalues so that $m < n$ implies $\lambda_m \le \lambda_n$, the *Weyl theorem* holds:

$$\lambda_n \sim \mathrm{meas}(\Omega) n^{\frac{2}{d}}, \qquad n \gg 1.$$

Moreover, the set $\{u_n \,:\, n \ge 0\}$ is dense in $\mathrm{L}(\Omega)$ (Courant & Hilbert 1962). All this creates grounds for a hope that the univariate theory of (Iserles & Nørsett 2006*a*) (and, indeed, of (Iserles & Nørsett 2006*b*)) might be generalised to a multivariate setting. In this paper we address this issue and argue that this hope is well grounded in reality. The univariate theory can indeed be comprehensively scaled up! Having said so, the more demanding framework calls upon substantially greater theoretical insight and algorithmic dexterity.

In Section 2 we introduce the multivariate theory. Thus, we determine the rate of decay of expansion coefficients and derive their asymptotic expansion. The latter is critical to an effective computation of the expansion. Our narrative is valid also in the case when the Laplacian is replaced by a polyharmonic operator and Neumann boundary conditions are of suitably high order but this is an approach that we do not pursue further in this paper.

The main obstacle in an implementation of the ideas of Section 2 is that we need to know the Laplace–Neumann spectrum *explicitly* in Ω. Even in a plane the set of domains where such information is available is currently restricted just to rectangles, ellipses, annuli and three types of triangles: equilateral, right triangle with two acute angles of $\frac{\pi}{4}$ and right triangle with acute angles of $\frac{\pi}{6}$ and $\frac{\pi}{3}$. The list is even shorter in higher dimensions.

Section 3 is concerned with the d-dimensional cube $[-1, 1]^d$, $d \ge 1$. This affords us an opportunity to flesh out details on the results of Section 2 and prepare the groundwork for the numerical work of Section 4. The case of the cube also highlights the crucial role played by integrals that oscillate only in some of the variables. Note that, on the face of it, stepping up from $[-1, 1]$ to $[-1, 1]^d$ by a Cartesian product is natural. Yet, it is neither necessarily easy nor straightforward and we need to get many details right.

The centrepiece of this paper is Section 4, devoted to the numerical computation of expansion coefficients using asymptotic and Filon-type techniques for highly oscillatory quadrature. Our goal is made more complicated because, as we have already observed, a significant proportion of expansion coefficients originate in integrals that oscillate only in some of their variables. This calls for a generalisation of an approach which we have dubbed "exotic quadrature" in (Iserles & Nørsett 2006*a*) and which is explained in detail in Section 5.

We note in passing that the number of coefficients required to approximate a function to given accuracy in a cube (or, for that matter, in other multivariate domains) can be reduced drastically once we observe that large coefficients assume the pattern of a *hyperbolic cross* (Babenko 1960). This phenomenon occurs also in Fourier and Chebyshev approximations, but it is less suitable for easy implementation in tandem with FFT techniques. Our asymptotics-based approach to the computation of expansion coefficients is just right for combination with the hyperbolic cross, and this leads to very substantial savings. Thus, in $[-1, 1]^d$, instead of computing $\mathcal{O}\bigl(N^d\bigr)$ expansion coefficients (where N represents required accuracy), we need to compute just $\mathcal{O}\bigl(N(\log_2 N)^{d-1}\bigr)$. We intend to examine this issue in considerably greater detail in a future paper.

The approach of Sections 3 and 4 lends itself to other domains in the plane where the Laplace–Neumann eigenfunctions are known, yet this requires substantial further effort. In a forthcoming paper we intend to discuss in great detail the case of $\Omega \subset \mathbb{R}^2$ being an equilateral triangle and its exploitation in the approximation of functions in arbitrary bounded bivariate polygonal domains. Another future paper will address acceleration techniques of expansions in Laplace–Neumann eigenfunctions.

2 Multivariate theory

Let $\Omega \subset \mathbb{R}^d$ be a simply-connected, bounded domain with piecewise-smooth boundary and assume that $u \in \mathrm{L}(\Omega)$ is an eigenfunction of the Laplace–Neumann problem in Ω, that is

$$-\Delta u = \lambda u, \quad \boldsymbol{x} \in \Omega, \qquad \frac{\partial u}{\partial n} = 0, \quad \boldsymbol{x} \in \partial\Omega. \tag{2.1}$$

We assume further that $\lambda \neq 0$ – as a matter of fact, in that case $\lambda > 0$, but this is irrelevant to the present argument. Given $f \in \mathrm{C}^\infty[\Omega]$, our concern is with $\langle f, u\rangle = \int_\Omega f u \mathrm{d}V$. Replacing u with $-\lambda^{-1}\Delta u$ and applying twice the Stokes theorem, we have

$$\begin{aligned}\langle f, u\rangle &= -\frac{1}{\lambda}\int_\Omega f(\boldsymbol{x})\Delta u(\boldsymbol{x})\mathrm{d}V = -\frac{1}{\lambda}\int_{\partial\Omega} f(\boldsymbol{x})\frac{\partial u(\boldsymbol{x})}{\partial n}\mathrm{d}S + \frac{1}{\lambda}\int_\Omega \nabla f(\boldsymbol{x})\cdot\nabla u(\boldsymbol{x})\mathrm{d}V\\ &= -\frac{1}{\lambda}\int_{\partial\Omega} f(\boldsymbol{x})\frac{\partial u(\boldsymbol{x})}{\partial n}\mathrm{d}S + \frac{1}{\lambda}\int_{\partial\Omega}\frac{\partial f(\boldsymbol{x})}{\partial n}u(\boldsymbol{x})\mathrm{d}S - \frac{1}{\lambda}\int_\Omega u(\boldsymbol{x})\Delta f(\boldsymbol{x})\mathrm{d}V.\end{aligned}$$

Substituting the Neumann boundary conditions, we thus deduce that

$$\langle f, u\rangle = \frac{1}{\lambda}\int_{\partial\Omega}\frac{\partial f(\boldsymbol{x})}{\partial n}u(\boldsymbol{x})\mathrm{d}S - \frac{1}{\lambda}\langle\Delta f, u\rangle. \tag{2.2}$$

We iterate (2.2),

$$\begin{aligned}\langle f, u\rangle &= \frac{1}{\lambda}\int_{\partial\Omega}\frac{\partial f(\boldsymbol{x})}{\partial n}u(\boldsymbol{x})\mathrm{d}S - \frac{1}{\lambda^2}\int_{\partial\Omega}\frac{\partial\Delta f(\boldsymbol{x})}{\partial n}u(\boldsymbol{x})\mathrm{d}S + \frac{1}{\lambda^2}\langle\Delta^2 f, u\rangle\\ &= \cdots = -\sum_{m=0}^{s}\frac{1}{(-\lambda)^{m+1}}\int_{\partial\Omega}\frac{\partial\Delta^m f(\boldsymbol{x})}{\partial n}u(\boldsymbol{x})\mathrm{d}S + \frac{1}{(-\lambda)^{s+1}}\langle\Delta^{s+1}f, u\rangle\end{aligned}$$

for any $s \in \mathbb{Z}_+$. Letting $s \to \infty$, we obtain the asymptotic expansion

$$\langle f, u\rangle \sim -\sum_{m=0}^{\infty}\frac{1}{(-\lambda)^{m+1}}\int_{\partial\Omega}\frac{\partial\Delta^m f(\boldsymbol{x})}{\partial n}u(\boldsymbol{x})\mathrm{d}S, \qquad \lambda \gg 1. \tag{2.3}$$

This expansion converges only in the asymptotic sense of the *Watson Lemma*. Yet, this is sufficient for the purposes of this paper since it demonstrates the pattern of dependence of $\langle f, u\rangle$ upon λ.

Note that this pattern is considerably more complicated than a naive look at (2.3) may imply. It is not just the λ^{-1} that matters but also the asymptotic behaviour of the integral $\int_{\partial\Omega}[\mathrm{d}f(\boldsymbol{x})/\mathrm{d}n]u(\boldsymbol{x})\mathrm{d}S$. For large λ the eigenfunction u is highly oscillatory, and this implies that the above integral is itself small – typically it can be also expanded in inverse powers of λ and the leading term is $\mathcal{O}(\lambda^{-\alpha})$, where $\alpha > 0$ depends upon critical points of u (Wong 2001). This, incidentally, is precisely the reason why the annihilation of the leading term,

$-\lambda^{-1}\int_{\partial\Omega} f(\boldsymbol{x})[\mathrm{d}u(\boldsymbol{x})/\mathrm{d}n]\mathrm{d}S$ is so important: since u oscillates rapidly, its normal derivative is large and the integral behaves like λ^{β} for some $\beta > 0$.

An illustration of both the importance and the limited utility of the asymptotic expansion (2.3) is provided by perhaps the simplest multivariate example, the square $\Omega = [-1, 1]^2$. In that case, to which we return with considerably greater generality and detail in Section 3, there are four kinds of eigenvalue–eigenfunction pairs, all conveniently labelled by a pair of indices,

$$\begin{aligned}
\lambda_{m,n}^{[0,0]} &= \pi^2(m^2+n^2), & u_{m,n}^{[0,0]}(x,y) &= \cos(\pi m x)\cos(\pi n y),\\
\lambda_{m,n}^{[0,1]} &= \pi^2[m^2+(n-\tfrac{1}{2})^2], & u_{m,n}^{[0,1]}(x,y) &= \cos(\pi m x)\sin[\pi(n-\tfrac{1}{2})y],\\
\lambda_{m,n}^{[1,0]} &= \pi^2[(m-\tfrac{1}{2})^2+n^2], & u_{m,n}^{[1,0]}(x,y) &= \sin[\pi(m-\tfrac{1}{2})x]\cos(\pi n y),\\
\lambda_{m,n}^{[1,1]} &= \pi^2[(m-\tfrac{1}{2})^2+(n-\tfrac{1}{2})^2], & u_{m,n}^{[1,1]}(x,y) &= \sin[\pi(m-\tfrac{1}{2})x]\sin[\pi(n-\tfrac{1}{2})y],
\end{aligned}$$

where the range of m and n is, for the time being, not important. Concentrating for the time being just on $u_{m,n}^{[1,1]}$, we note that each integral in (2.3) is a linear combination of four line integrals along the faces of the square, for example

$$\tfrac{1}{2}\int_{-1}^{1} g(x,1)\sin\pi(m-\tfrac{1}{2})x\mathrm{d}x.$$

This integral itself can be expanded asymptotically in inverse powers of m and it behaves like $\mathcal{O}(m^{-2})$ for $m \gg 1$ (Iserles & Nørsett 2006*a*). Combining this with (2.3), it follows in short order that

$$\langle f, u_{m,n}^{[1,1]}\rangle \sim \mathcal{O}\left(\frac{1}{m^2n^2}\right), \qquad m, n \gg 1.$$

For comparison, suppose that, in place of the Laplace–Neumann basis, we use the standard Fourier basis (more specifically, in a square, a Cartesian products of Fourier bases). This means the replacement of $u_{m,n}^{[1,1]}$ with

$$v_{m,n}^{[1,1]}(x,y) = \sin(\pi m x)\sin(\pi n y)$$

and it is easy to use the technique of (Iserles & Nørsett 2006*a*) to demonstrate that

$$\langle f, v_{m,n}^{[1,1]}\rangle \sim \mathcal{O}\left(\frac{1}{mn}\right), \qquad m, n \gg 1.$$

This underlies not just the speedup in convergence implicit in using Laplace–Neumann bases in preference to Fourier bases but also the role of the asymptotic expansion (2.3) in elucidating this phenomenon.

We cannot emphasise hard enough how important it is to consider the asymptotic behaviour of surface integrals in the determination of the overall decay of expansion coefficients in (2.3). An extreme example is provided by letting Ω be the bivariate unit disc, $\Omega = \{(x,y) : x^2+y^2 < 1\}$. It is an elementary exercise to prove that the Laplace–Neumann eigenfunctions are

$$u_{r,s}(x,y) = \mathrm{T}_r\left(\frac{y}{(x^2+y^2)^{\frac{1}{2}}}\right)\mathrm{J}_r(\mathrm{j}'_{r,s}(x^2+y^2)^{\frac{1}{2}}), \qquad r \in \mathbb{Z}_+, \quad s \in \mathbb{N}.$$

Here T_r is the r-degree Chebyshev polynomial, J_r is a Bessel function and $\mathrm{j}'_{r,s}$ is the sth positive zero of J'_r. The corresponding eigenvalue is $(\mathrm{j}'_{r,s})^2$. We deduce that

$$\int_{\partial\Omega} g(\boldsymbol{x})u_{r,s}(\boldsymbol{x})\mathrm{d}S = \frac{\mathrm{J}_n(\mathrm{j}'_{r,s})}{2\pi}\int_{-\pi}^{\pi} g(\cos\theta,\sin\theta)\cos r\theta\mathrm{d}\theta. \tag{2.4}$$

Provided that g is analytic in an annulus surrounding the unit circle, it follows that the above integral decays at an *exponential* rate, i.e. as $\mathrm{e}^{-\gamma r}$ for some $\gamma > 0$. (It can also be approximated rapidly and precisely by means of FFT, but we do not pursue this route in this paper.)

The disc is, in a sense, an exceptional case because the integral in (2.4) has no critical points. The unit cube, elaborated in some detail in Sections 3–5, is more typical.

Be it as it may, the expansion (2.3) provides the theoretical backdrop to expansions in Laplace–Neumann eigenfunctions and this is the right moment to introduce appropriate terminology and notation. We denote the countable set of Laplace–Neumann eigenvalues by λ_n, $n \in \mathbb{Z}_+$, where $\lambda_k \leq \lambda_n$ for $k < n$ (note that multiple eigenvalues are typical in this situation). A corresponding eigenfunction is denoted by u_n. Observe that $\lambda_0 = 0$ and, without loss of generality, $u_0 \equiv 1$. We recall from Section 1 the Weyl Theorem:

$$\lambda_n \sim \mathrm{meas}(\Omega)n^{\frac{2}{d}}, \qquad n \gg 1, \tag{2.5}$$

where $\mathrm{meas}(\Omega)$ is the measure of Ω.

Letting $\hat{f}_n = \langle f, u_n\rangle$ and $\hat{u}_n = \langle u_n, u_n\rangle$, $n \in \mathbb{Z}_+$, we consider the expansion of f in terms of the (dense in $\mathrm{L}[\Omega]$) basis of eigenfunctions,

$$\sum_{n=0}^{\infty} \frac{\hat{f}_n}{\hat{u}_n^{\frac{1}{2}}} u_n(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega. \tag{2.6}$$

It is eminently possible to combine the current approach with that of (Iserles & Nørsett 2006*b*) and consider, in place of the Laplace operator, a polyharmonic one. As an example – probably, the only realistic example in this setting – let u be an eigenfunction of the biharmonic–Neumann problem,

$$\Delta^2 u = \lambda u, \quad \boldsymbol{x} \in \Omega, \qquad \Delta u = \Delta\frac{\partial u}{\partial n} = 0, \quad \boldsymbol{x} \in \partial\Omega.$$

Proceeding as before, we apply the Stokes theorem four times, while substituting the zero Neumann boundary conditions. Thus,

$$\begin{aligned}\langle f, u\rangle &= \frac{1}{\lambda}\langle f, \Delta^2 u\rangle = \frac{1}{\lambda}\left(\int_{\partial\Omega} f\Delta\frac{\partial u}{\partial n} - \int_{\partial\Omega}\frac{\partial f}{\partial n}\Delta u + \langle \Delta f, \Delta u\rangle\right)\\ &= \frac{1}{\lambda}\langle \Delta f, \Delta u\rangle = \frac{1}{\lambda}\left[\int_{\partial\Omega}\Delta f\frac{\partial u}{\partial n} - \int_{\partial\Omega}\left(\Delta\frac{\partial f}{\partial n}\right)u + \langle \Delta^2 f, u\rangle\right].\end{aligned}$$

This can be iterated and the outcome is an expansion similar to (2.6). Note, however, that in the biharmonic case (2.5) is replaced by $\lambda_n \sim \mathrm{meas}(\Omega)n^{\frac{4}{d}}$, hence we can expect more rapid convergence – how rapid, needless to say, depends on critical points on u_n along $\partial\Omega$ and, as long as general theory is unavailable, need be examined on a case-by-case basis. We do not pursue this route in this paper since the Dirichlet–Neumann case is difficult enough, represents a raft of challenges and, clearly, its clarification must precede any elaboration of the polyharmonic case.

3 Eigenfunctions in the d-dimensional cube

In this section we discuss Laplace–Neumann bases in the d-dimensional cube $[-1,1]^d$ and present an asymptotic expansion of the corresponding expansion coefficients.

In principle, all we are doing is to generalise the univariate case, already considered in great detail in (Iserles & Nørsett 2006*a*), by using Cartesian products. Having said so, this generalisation is far from straightforward and is replete with fiddly details and special cases. This underlies the importance of getting the notation and terminology right.

It is instructive to commence from the univariate case, both to provide the starting point to an inductive argument and to introduce requisite notation in a fairly transparent and gentle manner. In the case $d = 1$ we have two families of eigenfunctions,

$$\cos \pi n x, \quad n \geq 0 \qquad \text{and} \qquad \sin \pi (n - \tfrac{1}{2}) x, \quad n \geq 1$$

and the modified Fourier expansion of $f \in \mathrm{L}[-1,1]$ is

$$\tfrac{1}{2} \hat{f}_0^{[0]} + \sum_{n=1}^{\infty} [\hat{f}_n^{[0]} \cos \pi n x + \hat{f}_n^{[1]} \sin \pi (n - \tfrac{1}{2}) x], \tag{3.1}$$

where

$$\hat{f}_n^{[0]} = \int_{-1}^{1} f(x) \cos(\pi n x) \mathrm{d}x, \qquad \hat{f}_n^{[1]} = \int_{=1}^{1} f(x) \sin[\pi (n - \tfrac{1}{2}) x] \mathrm{d}x.$$

Our first observation is that a single integral, $\hat{f}_0^{[0]}$, is exceptional, both because it is non-oscillatory and since it is scaled by $\frac{1}{2}$. We say that it is of *grade* 0 and designate remaining integrals to be of grade 1. The coefficients $\hat{f}_n^{[0]}$ and $\hat{f}_n^{[1]}$ have been expanded asymptotically in (Iserles & Nørsett 2006*a*): for any $f \in \mathrm{C}^\infty[-1,1]$ it is true that

$$\hat{f}_n^{[0]} \sim (-1)^n \sum_{m=0}^{\infty} \frac{(-1)^m}{(\pi n)^{2m+2}} [f^{(2m+1)}(1) - f^{(2m+1)}(-1)],$$

$$\hat{f}_n^{[1]} \sim (-1)^{n-1} \sum_{m=0}^{\infty} \frac{(-1)^m}{[\pi (n - \frac{1}{2})]^{2m+2}} [f^{(2m+1)}(1) + f^{(2m+1)}(-1)], \qquad n \gg 1.$$

To write (3.1) in a manner which is more convenient for multivariate work we let

$$\mu_n^{[0]} = n, \quad \mu_n^{[1]} = n - \tfrac{1}{2}, \qquad c_n^{[j]} = \begin{cases} \frac{1}{2}, & n = 0,\ j = 0, \\ 0, & n = 0,\ j = 1, \\ 1, & n \geq 1,\ j \in \{0,1\}, \end{cases}$$

and set

$$u_n^{[0]}(x) = \cos \pi n x, \qquad u_n^{[1]}(x) = \sin \pi (n - \tfrac{1}{2}) x.$$

Therefore the expansion (3.1) can be written succinctly in the form

$$\sum_{m=0}^{\infty} \sum_{j=0}^{1} c_m^{[j]} \hat{f}_m^{[j]} u_m^{[j]}(x), \tag{3.2}$$

where

$$\hat{f}_n^{[j]} \sim (-1)^{n+j} \sum_{m=0}^{\infty} \frac{(-1)^m}{(\pi\mu_n^{[j]})^{2m+2}} [f^{(2m+1)}(1) - (-1)^j f^{(2m+1)}(-1)], \qquad n \gg 1. \quad (3.3)$$

We next consider the multivariate case $d \geq 1$: our aim is to generalise the expansion (3.2) and the asymptotic formula (3.3). Let $\mathbb{Z}_2^d$ be the set of all the d-tuples of binary numbers and $\mathbb{Z}_+^d$ the set of d-tuples of nonnegative integers. We employ multi-index notation, in particular

$$|\boldsymbol{e}| = \sum_{k=1}^{d} e_k, \qquad \partial_{\boldsymbol{x}}^{\boldsymbol{m}} = \partial_{x_1}^{m_1} \partial_{x_2}^{m_2} \cdots \partial_{x_d}^{m_d}.$$

For every $\boldsymbol{y} \in [-1,1]^d$ and $\boldsymbol{\alpha} \in \mathbb{Z}_2^d$ we define

$$\mathcal{S}_{\boldsymbol{\alpha}}[f](\boldsymbol{y}) = \sum_{\boldsymbol{e} \in \mathbb{Z}_2^d} (-1)^{|\boldsymbol{e}| + \boldsymbol{e}^\top \boldsymbol{\alpha}} f((-1)^{e_1} y_1, (-1)^{e_2} y_2, \ldots, (-1)^{e_d} y_d).$$

Theorem 1 *The Laplace–Neumann eigenfunctions in $[-1,1]^d$ are*

$$u_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]}(\boldsymbol{x}) = \prod_{j=1}^{d} u_{n_j}^{[\alpha_j]}(x_j), \qquad n_j \geq \alpha_j, \quad j = 1, \ldots, d, \qquad \boldsymbol{\alpha} \in \mathbb{Z}_2^d \quad (3.4)$$

and it is true that (in the Euclidean norm) $\|u_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]}\| = 1$. Moreover, the expansion of $f \in \mathrm{C}^\infty[-1,1]^d$ is

$$\sum_{\boldsymbol{n} \in \mathbb{Z}_+^d} \sum_{\boldsymbol{\alpha} \in \mathbb{Z}_2^d} c_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]} \hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]} u_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]}(\boldsymbol{x}), \quad (3.5)$$

where

$$c_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]} = \begin{cases} 0, & \exists j \in \boldsymbol{\chi}(\boldsymbol{n}) \text{ such that } \alpha_j = 1, \\ 2^{-\#\boldsymbol{\chi}(\boldsymbol{n})}, & \text{otherwise,} \end{cases}$$

where $\boldsymbol{\chi}(\boldsymbol{n}) = \{i : n_i = 0\}$ and $\#S$ is the number of terms in the set S, while

$$\hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]} = \int_{[-1,1]^d} f(\boldsymbol{x}) u_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]}(\boldsymbol{x}) \mathrm{d}x_1 \cdots \mathrm{d}x_d.$$

Proof It is clear by inspection that (3.4) are the eigenfunctions, forming a Cartesian product of univariate eigenfunctions. Moreover,

$$\|u_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]}\|^2 = \prod_{j=1}^{d} \int_{-1}^{1} {u_{n_j}^{[\alpha_j]}}^2(x_j) \mathrm{d}x_j = 1,$$

because the univariate eigenfunctions are of unit norm. The remainder of the theorem is an immediate consequence of a Cartesian product of (3.2). □

In line with the univariate setting, we say that $\hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]}$ is of *grade* $d - \#\chi(n)$. Intuitively speaking, grade s means that, for $n_1, \ldots, n_d \gg 1$, the eigenfunction $u_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]}$ is oscillatory in s variables.

Theorem 2 *Each coefficient* $\hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]}$ *has the asymptotic expansion*

$$\hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]} \sim (-1)^{|\boldsymbol{n}|+|\boldsymbol{\alpha}|} \sum_{m=0}^{\infty} \frac{(-1)^m}{\pi^{2m+2d}} \sum_{|\boldsymbol{j}|=m} \frac{\mathcal{S}_{\boldsymbol{\alpha}}[\partial_{\boldsymbol{x}}^{2\boldsymbol{j}+\mathbf{1}} f](\mathbf{1})}{\mu_{n_1}^{[\alpha_1]\,2j_1+2} \cdots \mu_{n_d}^{[\alpha_d]\,2j_d+2}}, \qquad n_1,\ldots,n_d \gg 1. \tag{3.6}$$

Proof By induction on d. For $d = 1$ (3.6) coincides with (3.3). Assuming that it is correct for $d-1$, we apply the asymptotic expansion to the first $d-1$ coordinates: exchanging summation and integration whenever necessary, we have

$$\hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]} \sim (-1)^{|\tilde{\boldsymbol{n}}|+|\tilde{\boldsymbol{\alpha}}|} \sum_{m=0}^{\infty} \frac{(-1)^m}{\pi^{2m+2d-2}} \sum_{|\tilde{\boldsymbol{\jmath}}|=m} \frac{1}{\mu_{n_1}^{[\alpha_1]\,2j_1+2} \cdots \mu_{n_{d-1}}^{[\alpha_{d-1}]\,2j_{d-1}+2}}$$
$$\times \int_{-1}^{1} \mathcal{S}_{\tilde{\boldsymbol{\alpha}}}[\partial_{\boldsymbol{x}}^{2\tilde{\boldsymbol{\jmath}}+\mathbf{1}} f](1,\ldots,1,x_d)\, u_{n_d}^{[\alpha_d]}(x_d)\,\mathrm{d}x_d, \qquad n_1,\ldots,n_{d-1} \gg 1,$$

where

$$\tilde{\boldsymbol{\alpha}} = [\ \alpha_1 \quad \alpha_2 \quad \cdots \quad \alpha_{d-1}\ ] \qquad \text{and} \qquad \tilde{\boldsymbol{\jmath}} = [\ j_1 \quad j_2 \quad \cdots \quad j_{d-1}\ ].$$

Applying (3.3) to the univariate integral in the last expansion, we obtain

$$\int_{-1}^{1} \mathcal{S}_{\tilde{\boldsymbol{\alpha}}}[\partial_{\boldsymbol{x}}^{2\tilde{\boldsymbol{\jmath}}+\mathbf{1}} f](1,\ldots,1,x_d)\, u_{n_d}^{[\alpha_d]}(x_d)\,\mathrm{d}x_d$$
$$\sim (-1)^{n_d+\alpha_d} \sum_{j_d=0}^{\infty} \frac{(-1)^{j_d}}{(\pi\mu_{n_d}^{[\alpha_d]})^{2j_d+2}} [\partial_{x_d}^{2j_d+1} f(1,\ldots,1) - (-1)^{\alpha_d} \partial_{x_d}^{2j_d+1} f(1,\ldots,1,-1)].$$

Therefore,

$$\hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]} \sim (-1)^{|\boldsymbol{n}|+|\boldsymbol{\alpha}|} \sum_{m=0}^{\infty} \sum_{j_d=0}^{\infty} \frac{(-1)^{m+j_d}}{\pi^{2m+2j_d+2d}} \sum_{|\tilde{\boldsymbol{\jmath}}|=m} \frac{1}{\mu_{n_1}^{[\alpha_1]\,2j_1+2} \cdots \mu_{n_{d-1}}^{[\alpha_{d-1}]\,2j_{d-1}+2}\ \mu_{n_d}^{[\alpha_d]\,2j_d+2}}$$
$$\times \{\mathcal{S}_{\tilde{\boldsymbol{\alpha}}}[\partial_{\boldsymbol{x}}^{2\tilde{\boldsymbol{\jmath}}+\mathbf{1}} \partial_{x_d}^{2j_d+1} f](1,\ldots,1) - (-1)^{\alpha_d} \mathcal{S}_{\tilde{\boldsymbol{\alpha}}}[\partial_{\boldsymbol{x}}^{2\tilde{\boldsymbol{\jmath}}+\mathbf{1}} \partial_{x_d}^{2j_d+1} f](1,\ldots,1,-1)\}.$$

However, it follows at once from the definition of $\mathcal{S}_{\boldsymbol{\alpha}}$ that

$$\begin{aligned}
&\mathcal{S}_{\boldsymbol{\alpha}}[\partial_{\boldsymbol{x}}^{2\boldsymbol{j}+\mathbf{1}} f](\boldsymbol{y}) \\
&= \sum_{\tilde{\boldsymbol{e}} \in \mathbb{Z}_2^{d-1}} (-1)^{|\tilde{\boldsymbol{e}}|+\tilde{\boldsymbol{e}}^\top \tilde{\boldsymbol{\alpha}}} \partial_{\boldsymbol{x}}^{2\boldsymbol{j}+1} f((-1)^{e_1} y_1,\ldots,(-1)^{e_{d-1}} y_{d-1}, y_d) \\
&\quad - (-1)^{\alpha_d} \sum_{\tilde{\boldsymbol{e}} \in \mathbb{Z}_2^{d-1}} (-1)^{|\tilde{\boldsymbol{e}}|+\tilde{\boldsymbol{e}}^\top \tilde{\boldsymbol{\alpha}}} \partial_{\boldsymbol{x}}^{2\boldsymbol{j}+1} f((-1)^{e_1} y_1,\ldots,(-1)^{e_{d-1}} y_{d-1}, -y_d) \\
&= \mathcal{S}_{\tilde{\boldsymbol{\alpha}}}[\partial_{\boldsymbol{x}}^{2\tilde{\boldsymbol{\jmath}}+\mathbf{1}} \partial_{x_d}^{2j_d+1} f](\tilde{\boldsymbol{y}}, y_d) - (-1)^{\alpha_d} \mathcal{S}_{\tilde{\boldsymbol{\alpha}}}[\partial_{\boldsymbol{x}}^{2\tilde{\boldsymbol{\jmath}}+\mathbf{1}} \partial_{x_d}^{2j_d+1} f](\tilde{\boldsymbol{y}}, -y_d).
\end{aligned}$$

We conclude that

$$\hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]} \sim (-1)^{|\boldsymbol{n}|+|\boldsymbol{\alpha}|} \sum_{m=0}^{\infty} \sum_{j_d=0}^{\infty} \frac{(-1)^{m+j_d}}{\pi^{2m+2j_d+2d}} \sum_{|\tilde{\boldsymbol{\jmath}}|=m} \frac{\mathcal{S}_{\boldsymbol{\alpha}}[\partial_{\boldsymbol{x}}^{2\boldsymbol{j}+\mathbf{1}} f](\mathbf{1})}{\mu_{n_1}^{[\alpha_1]\,2j_1+2} \cdots \mu_{n_d}^{[\alpha_d]\,2j_d+2}}$$

$$= (-1)^{|\boldsymbol{n}|+|\boldsymbol{\alpha}|} \sum_{j_d=0}^{\infty} \sum_{m=j_d}^{\infty} \frac{(-1)^m}{\pi^{2m+2d}} \sum_{|\tilde{\boldsymbol{\jmath}}|=m-j_d} \frac{\mathcal{S}_{\boldsymbol{\alpha}}[\partial_{\boldsymbol{x}}^{2\boldsymbol{j}+\boldsymbol{1}} f](\boldsymbol{1})}{\mu_{n_1}^{[\alpha_1]\,2j_1+2} \cdots \mu_{n_d}^{[\alpha_d]\,2j_d+2}}$$

$$= (-1)^{|\boldsymbol{n}|+|\boldsymbol{\alpha}|} \sum_{m=0}^{\infty} \frac{(-1)^m}{\pi^{2m+2d}} \sum_{j_d=0}^{m} \sum_{|\tilde{\boldsymbol{\jmath}}|+j_d=m} \frac{\mathcal{S}_{\boldsymbol{\alpha}}[\partial_{\boldsymbol{x}}^{2\boldsymbol{j}+\boldsymbol{1}} f](\boldsymbol{1})}{\mu_{n_1}^{[\alpha_1]\,2j_1+2} \cdots \mu_{n_d}^{[\alpha_d]\,2j_d+2}}$$

$$= (-1)^{|\boldsymbol{n}|+|\boldsymbol{\alpha}|} \sum_{m=0}^{\infty} \frac{(-1)^m}{\pi^{2m+2d}} \sum_{|\boldsymbol{j}|=m} \frac{\mathcal{S}_{\boldsymbol{\alpha}}[\partial_{\boldsymbol{x}}^{2\boldsymbol{j}+\boldsymbol{1}} f](\boldsymbol{1})}{\mu_{n_1}^{[\alpha_1]\,2j_1+2} \cdots \mu_{n_d}^{[\alpha_d]\,2j_d+2}},$$

which is (3.6). □

To illustrate the last two theorems we let $d = 2$ and $f(x, y) = \mathrm{e}^{x-2y}$. This very simple function has the virtue of leading to explicit and exceedingly simple expressions which, with some persistence, can be verified directly. Thus,

$$\hat{f}_{m,n}^{[0,0]} = \int_{-1}^{1}\int_{-1}^{1} \mathrm{e}^{x-2y} \cos(\pi m x) \cos(\pi n y) \mathrm{d}x \mathrm{d}y = \frac{2(-1)^{m+n}\gamma^{[0,0]}}{(1+\pi^2 m^2)(4+\pi^2 n^2)},$$

$$\hat{f}_{m,n}^{[0,1]} = \int_{-1}^{1}\int_{-1}^{1} \mathrm{e}^{x-2y} \cos(\pi m x) \sin[\pi(n-\tfrac{1}{2})y] \mathrm{d}x \mathrm{d}y = \frac{2(-1)^{m+n}}{(1+\pi^2 m^2)[4+\pi^2 (n-\frac{1}{2})^2]},$$

$$\hat{f}_{m,n}^{[1,0]} = \int_{-1}^{1}\int_{-1}^{1} \mathrm{e}^{x-2y} \sin[\pi(m-\tfrac{1}{2})x] \cos(\pi n y) \mathrm{d}x \mathrm{d}y = \frac{2(-1)^{m+n-1}\gamma^{[1,0]}}{[1+\pi^2 (m-\frac{1}{2})^2](4+\pi^2 n^2)},$$

$$\hat{f}_{m,n}^{[1,1]} = \int_{-1}^{1}\int_{-1}^{1} \mathrm{e}^{x-2y} \sin[\pi(m-\tfrac{1}{2})x] \sin[\pi(n-\tfrac{1}{2})y] \mathrm{d}x \mathrm{d}y$$

$$= \frac{2(-1)^{m+n-1}\gamma^{[1,1]}}{[1+\pi^2 (m-\frac{1}{2})^2][4+\pi^2 (n-\frac{1}{2})^2]}$$

where

$$\gamma^{[0,0]} = (\mathrm{e}^2-1)(\mathrm{e}-\mathrm{e}^{-3}), \qquad \gamma^{[0,1]} = (\mathrm{e}^2-1)(\mathrm{e}+\mathrm{e}^{-3}),$$
$$\gamma^{[1,0]} = (\mathrm{e}^2+1)(\mathrm{e}-\mathrm{e}^{-3}), \qquad \gamma^{[1,1]} = (\mathrm{e}^2+1)(\mathrm{e}+\mathrm{e}^{-3})$$

and the corresponding asymptotic expansions are

$$\hat{f}_{m,n}^{[0,0]} \sim \frac{2(-1)^{m+n}\gamma^{[0,0]}}{\pi^4 m^2 n^2} - \frac{2(-1)^{m+n}\gamma^{[0,0]}}{\pi^6} \left(\frac{4}{m^2 n^4} + \frac{1}{m^4 n^2}\right) + \cdots,$$

$$\hat{f}_{m,n}^{[0,1]} \sim \frac{2(-1)^{m+n}\gamma^{[0,1]}}{\pi^4 m^2 (n-\frac{1}{2})^2} - \frac{2(-1)^{m+n}\gamma^{[0,1]}}{\pi^6} \left[\frac{4}{m^2 (n-\frac{1}{2})^4} + \frac{1}{m^4 (n-\frac{1}{2})^2}\right] + \cdots,$$

$$\hat{f}_{m,n}^{[1,0]} \sim \frac{2(-1)^{m+n-1}\gamma^{[1,0]}}{\pi^4 (m-\frac{1}{2})^2 n^2} - \frac{2(-1)^{m+n-1}\gamma^{[1,0]}}{\pi^6} \left[\frac{4}{(m-\frac{1}{2})^2 n^4} + \frac{1}{(m-\frac{1}{2})^4 n^2}\right] + \cdots,$$

$$\hat{f}_{m,n}^{[1,1]} \sim \frac{2(-1)^{m+n-1}\gamma^{[1,1]}}{\pi^4 (m-\frac{1}{2})^2 (n-\frac{1}{2})^2} - \frac{2(-1)^{m+n-1}\gamma^{[1,1]}}{\pi^6} \left[\frac{4}{(m-\frac{1}{2})^2 (n-\frac{1}{2})^4} + \frac{1}{(m-\frac{1}{2})^4 (n-\frac{1}{2})^2}\right] + \cdots.$$

This is the place to discuss briefly issues of convergence. It has been proved in (Iserles & Nørsett 2006*a*) that the univariate modified Fourier expansion of a Lipschitz function converges uniformly in any closed subinterval of $(-1, 1)$ where it is continuous. Moreover, if f is analytic in an open complex domain inclusive of $[-1, 1]$ then the expansion converges at the endpoints: this is an example of superiority of modified over conventional Fourier expansions in this setting, since the latter fail to converge there unless f is periodic. The speed of convergence is also of interest. It has been proved in (Iserles & Nørsett 2006*a*) that an N-term expansion converges at ± 1 as $\mathcal{O}(N^{-1})$ and it was conjectured there that, subject to sufficient smoothness of f, the convergence in $(-1, 1)$ is at the rate of $\mathcal{O}(N^{-2})$ (compare to the $\mathcal{O}(n^{-1})$ rate of conventional Fourier!). This has been recently proved by Olver (2007).

The above rate of convergence can be generalised from $[-1, 1]$ to the d-dimensional cube $[-1, 1]^d$ at once by means of a Cartesian product. This is illustrated in Fig. 3.1. It is easy to observe that the error is substantially larger on the boundary and, perhaps unsurprisingly, it reaches its peak at $(1, -1)$, the maximum of f. Doubling N halves the error along the boundary but it decreases it roughly by a factor of four inside the square, in line with the theory in (Olver 2007).

4 Quadrature in the d-dimensional cube

Laplace–Neumann eigenfunctions oscillate rapidly, consequently modified Fourier coefficients are integrals with highly oscillatory kernels. This allows us to use in the current setting powerful and affordable *Filon-type* techniques for highly oscillatory quadrature which have been originally developed in (Iserles & Nørsett 2005). This has been accomplished in (Iserles & Nørsett 2006*a*) for the univariate expansion and it is instructive to commence by discussing the additional constraints imposed by current imperatives, as compared with standard highly oscillatory quadrature.

Firstly, we need an efficient approach not just to evaluate a single highly oscillatory integral but a large number of coefficients $\hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]}$: except for $\boldsymbol{n} = \boldsymbol{0}$, all these are distinct oscillatory integrals. All modern methods for highly oscillatory quadrature require the computation of f and its derivatives at a number of points – clearly, in the current situation we wish to avoid repeated computation of function values for each $\boldsymbol{n}$ within the relevant range. Instead, we will compute function values and derivatives only once and recycle them repeatedly for each $\boldsymbol{n}$.

Secondly, not all integrands oscillate rapidly and not all oscillations are alike. Specifically, we need to pay attention to the grade s of each $\hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]}$. Since the underlying eigenfunction $u_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]}$ oscillates in just s variables and is non-oscillatory in the remaining $d - s$, we need to apply highly oscillatory quadrature techniques to just s variables and otherwise use classical quadrature. Except that the imperative of reusing the same function and derivative information for all $\boldsymbol{n}$ and $\boldsymbol{\alpha}$ impose restrictions on the non-oscillatory quadrature. Classical quadrature, in particular Gaussian quadrature, is not longer adequate. We are instead compelled to develop new non-oscillatory quadrature techniques, which we have dubbed "exotic quadrature" in (Iserles & Nørsett 2006*a*).

Both above issues have been addressed comprehensively in a univariate setting in (Iserles & Nørsett 2006*a*, Iserles & Nørsett 2006*b*) but in the multivariate case we are faced with additional challenges which a naive Cartesian product falls short of solving.

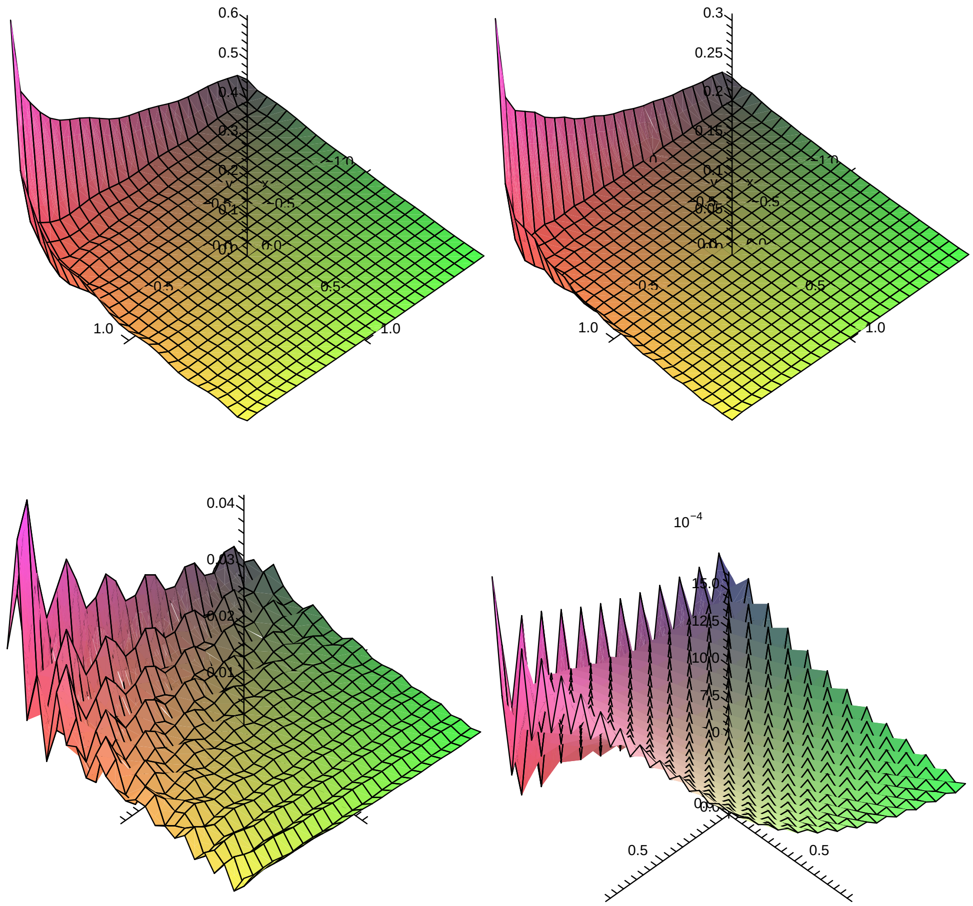


Figure 3.1: The absolute error in approximating e^{x-2y} by the truncated expansion (3.5), with $n_1, n_2 \le N$. In the top row we approximate in $[-1,1]^2$ with $N = 20$ and $N = 40$ respectively, while the bottom row reports the same information in the cube $[-\frac{9}{10}, \frac{9}{10}]^2$.

4.1 Asymptotic methods

The obvious approach to the computation of the coefficients $\hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]}$ is to truncate the asymptotic expansion (3.6). This results in the *asymptotic method*

$$\mathcal{A}_{\boldsymbol{n},N}^{[\boldsymbol{\alpha}]} = (-1)^{|\boldsymbol{n}|+|\boldsymbol{\alpha}|} \sum_{m=0}^{N-1} \frac{(-1)^m}{\pi^{2m+2d}} \sum_{|\boldsymbol{j}|=m} \frac{\mathcal{S}_{\boldsymbol{\alpha}}[\partial_{\boldsymbol{x}}^{2\boldsymbol{j}+\boldsymbol{1}} f](\boldsymbol{1})}{\mu_{n_1}^{[\alpha_1]\,2j_1+2} \cdots \mu_{n_d}^{[\alpha_d]\,2j_d+2}}, \tag{4.1}$$

where $N \in \mathbb{N}$. It is well-defined for $n_1, \ldots, n_d \ge 1$ and makes sense when $n_1, \ldots, n_d$ are sufficiently large.

$\boldsymbol{n}$	$\boldsymbol{\alpha}$	$\mathcal{A}_{\boldsymbol{n},1}^{[\boldsymbol{\alpha}]}$	$\mathcal{A}_{\boldsymbol{n},2}^{[\boldsymbol{\alpha}]}$	$\mathcal{A}_{\boldsymbol{n},3}^{[\boldsymbol{\alpha}]}$	$\mathcal{A}_{\boldsymbol{n},4}^{[\boldsymbol{\alpha}]}$
$[1,1]$	$[0,0]$	1.2387_{-01}	5.3467_{-02}	2.2000_{-02}	8.9497_{-03}
	$[1,0]$	9.0754_{-01}	5.8271_{-01}	3.2326_{-01}	1.6631_{-01}
	$[0,1]$	9.4931_{-01}	1.5525_{+00}	2.5182_{+00}	4.0825_{+01}
	$[1,1]$	5.5575_{+00}	9.9012_{+00}	1.6428_{+01}	2.6753_{+01}
$[2,3]$	$[0,0]$	6.4873_{-04}	3.5305_{-05}	1.7440_{-06}	8.2437_{-08}
	$[1,0]$	1.9140_{-03}	1.3024_{-04}	7.8481_{-06}	4.4273_{-07}
	$[0,1]$	1.2215_{-03}	8.8296_{-05}	5.9558_{-06}	3.9204_{-07}
	$[1,1]$	3.4367_{-02}	2.8864_{-04}	2.1680_{-05}	1.5393_{-06}
$[7,4]$	$[0,0]$	1.1929_{-05}	3.0407_{-07}	7.7062_{-09}	1.9521_{-10}
	$[1,0]$	1.8384_{-05}	4.6957_{-07}	1.1904_{-08}	3.0155_{-10}
	$[0,1]$	2.0581_{-05}	6.8351_{-07}	2.2688_{-08}	7.4834_{-10}
	$[1,1]$	3.1635_{-05}	1.0519_{-06}	3.4816_{-08}	1.1519_{-09}
$[10,10]$	$[0,0]$	1.7659_{-07}	7.5158_{-10}	3.0824_{-12}	1.2529_{-14}
	$[1,0]$	2.6245_{-07}	1.1278_{-09}	4.6428_{-12}	1.8897_{-14}
	$[0,1]$	2.2041_{-07}	1.0311_{-09}	4.6721_{-12}	2.1023_{-14}
	$[1,1]$	3.2704_{-07}	1.5423_{-09}	7.0089_{-12}	3.1568_{-14}

Table 1: Absolute value of the errors, $|\mathcal{A}_{\boldsymbol{n},N}^{[\boldsymbol{\alpha}]} - \hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]}|$, committed by different asymptotic methods, four different $\boldsymbol{n}$s and $f(x,y) = \mathrm{e}^{x-2y}$.

Lemma 3 *Let $\bar{n} = \min\{n_1, \ldots, n_d\}$. Then*

$$\mathcal{A}_{\boldsymbol{n},N}^{[\boldsymbol{\alpha}]} \sim \hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]} + \mathcal{O}\left(\bar{n}^{-2(N+d)}\right), \qquad \bar{n} \gg 1. \tag{4.2}$$

Proof Follows immediately by comparing (3.6) and (4.1). □

Before contemplating further the method (4.1), it is important to observe that its implementation is *linear* in the number of coefficients, once we precompute $\partial_{\boldsymbol{x}}^{2\boldsymbol{n}+\mathbf{1}} f$, $0 \leq |\boldsymbol{n}| \leq N-1$, at the 2^d vertices of the cube. This fulfils our first goal, yet (4.1) clearly falls short of delivering useful approximation for terms of grades $\leq d-1$ and, indeed, for small $\bar{n}$. Without disregarding this important issue, we defer its discussion for the time being.

Both advantages and disadvantages of the asymptotic method (4.1) are apparent from Table 1. Its performance is poor for ‘small’ $\boldsymbol{n}$s: it either diverges or converges very slowly and incurs unacceptably large error. Yet, that very ‘smallness’, which depends on the function f, is deceptive. Asymptotic behaviour kicks in for fairly moderate values of $\bar{n}$. Thus, $\bar{n} = 2$ is already within convergent regime, albeit perhaps too slow for our needs.

Having said so, the lesson of recent work on highly oscillatory quadrature and modified Fourier expansions is that the great virtue of an asymptotic expansion is often not as a numerical method *per se*, but as a theoretical device underlying and underpinning more effective numerical methods. This is the subject of the next subsection.

4.2 Filon-type methods

Let ψ be a sufficiently smooth function defined in $[-1,1]^d$ and such that

$$\partial_{\boldsymbol{x}}^{2\boldsymbol{m}+1}\psi((-1)^{\boldsymbol{e}}) = \partial_{\boldsymbol{x}}^{2\boldsymbol{m}+1} f((-1)^{\boldsymbol{e}}), \qquad |\boldsymbol{m}| \le N-1, \quad \boldsymbol{e} \in \mathbb{Z}_+^d. \tag{4.3}$$

In other words, the odd derivatives of ψ and f of degree $\le 2N-1$ match at all the corners of the cube. This results in $2^d \sum_{j=0}^{N-1} \binom{d+2j}{d-1} \approx 2^{2d-1} N^d / d!$ conditions. Our underlying assumption is that the expansion coefficients corresponding to the function ψ,

$$\mathcal{Q}_{\boldsymbol{n},N}^{[\boldsymbol{\alpha}]} = \hat{\psi}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]}, \tag{4.4}$$

can be calculated explicitly. This is certainly the case when ψ is a d-variable polynomial, an approach which we adopt herewith. (Note that interesting non-polynomial choices of ψ, in a different context, have been recently discussed in (Olver 2006*a*), but we do not follow this route in the current paper.)

The approximation (4.4) is an elementary example of a *Filon-type method* (Iserles & Nørsett 2005) and it is usual to augment (4.3) with additional interpolation conditions. Thus, in full generality, we choose $s \ge 2^d$ *quadrature points* $\boldsymbol{c}_k$ in $[-1,1]^d$, the first 2^d of which are the vertices. In addition, we choose s *index sets*

$$\mathcal{D}_k = \{\boldsymbol{i}_{k,1}, \boldsymbol{i}_{k,2}, \ldots, \boldsymbol{i}_{k,m_k}\}, \qquad k = 1,\ldots,s,$$

where $\boldsymbol{i}_{k,j} \in \mathbb{Z}_+^d$. For each $1 \le k \le 2^d$ we stipulate that

$$\{\boldsymbol{i} \in \mathbb{Z}_+ : |\boldsymbol{i}| \le N-1\} \subseteq \mathcal{D}_k.$$

We choose a polynomial ψ that satisfies the interpolation conditions

$$\partial_{\boldsymbol{x}}^{\boldsymbol{i}_{k,j}} \psi(\boldsymbol{c}_k) = \partial_{\boldsymbol{x}}^{\boldsymbol{i}_{k,j}} f(\boldsymbol{c}_k), \qquad j = 1,\ldots,m_k, \quad k = 1,\ldots,s, \tag{4.5}$$

and note that (4.3) is a subset of (4.5). The corresponding Filon-type method is defined by (4.4).

Lemma 4 *Given a Filon-type method (4.4) and subject to the interpolation conditions (4.5), it is true that*

$$\mathcal{Q}_{\boldsymbol{n},N}^{[\boldsymbol{\alpha}]} \sim \hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]} + \mathcal{O}\left(\bar{n}^{-2(N+d)}\right), \qquad \bar{n} \gg 1.$$

Proof Follows at once by letting $\psi - f$ in place of f in the asymptotic formula (4.1) and using the interpolation condition (4.3). □

Note that (4.5) represents $m^\star = \sum_{k=1}^s m_k$ interpolation conditions. Choosing a suitable d-variate polynomial ψ with the right number of degrees of freedom is one of the main challenges in the design of Filon-type methods for modified Fourier expansions in a cube. Note further that the relationship between the number $m^\star$ of interpolations conditions and the number of degrees of freedom $r^\star$, say, in the polynomial basis is in general unclear. Clearly, we require $r^\star \ge m^\star$, but for general conditions (4.5) we might require $r^\star$ to be larger (possibly, much larger) than $m^\star$. There are two possible obstacles to our construction and we must discuss them both.

Firstly – and this phenomenon occurs already for $d = 1$ – (4.3) is a so-called *Birkhoff–Hermite interpolation problem* (Lorenz, Jetter & Riemenschneider 1983): we interpolate to non-consecutive derivatives and we cannot take it for granted that this can be done with $r^\star = m^\star$. Secondly, multivariate polynomial interpolation (even Lagrangian interpolation, to say nothing of the Birkhoff–Hermite kind) need not exist for a particular configuration of interpolation points and conditions (4.5) in a multivariate setting.

A comparison of Lemma 3 and 4 allows for an alternative interpretation of Filon-type methods in the current setting, which we have already considered in the univariate case in (Iserles & Nørsett 2006*a*) and which we will find very useful indeed in the next subsection. Thus,

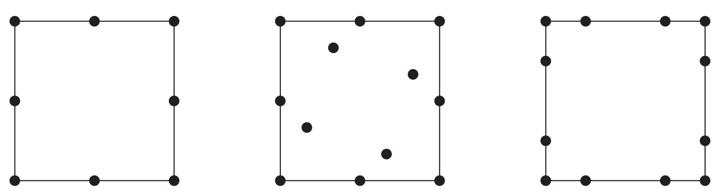
$$\begin{aligned}\mathcal{Q}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},N} &= \mathcal{A}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},N} + \mathcal{O}\left(\bar{n}^{-2(N+d)}\right) \qquad (4.6)\\ &= \mathcal{A}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},N} + \frac{(-1)^{|\boldsymbol{n}|+|\boldsymbol{\alpha}|+N}}{\pi^{2(N+d)}} \sum_{|\boldsymbol{j}|=N} \frac{\mathcal{E}^{[\boldsymbol{\alpha}]}_{\boldsymbol{j}}[f]}{\mu^{[\alpha_1]\,2j_1+2}_{n_1} \cdots \mu^{[\alpha_d]\,2j_d+2}_{n_d}} + \mathcal{O}\left(\bar{n}^{-2(N+d+1)}\right)\end{aligned}$$

and, comparing with (3.6), we interpret $\mathcal{E}^{[\boldsymbol{\alpha}]}_{\boldsymbol{j}}[f]$ as an approximation to $\mathcal{S}_{\boldsymbol{\alpha}}[\partial^{2\boldsymbol{j}+\boldsymbol{1}}_{\boldsymbol{x}} f](\boldsymbol{1})$. Therefore, we abandon altogether the interpretation of the Filon-type method as the integral where f has been replaced by an interpolating polynomial ψ, subject to the conditions (4.5). Instead, we seek coefficients $\sigma^{[\boldsymbol{\alpha}]}_{\boldsymbol{j}}(k,j)$, where $|\boldsymbol{j}| = N$, $j = 1,\ldots,m_k$, $k = 1,\ldots,s$, so that

$$\mathcal{E}^{[\boldsymbol{\alpha}]}_{\boldsymbol{j}}[g] = \sum_{k=1}^{s} \sum_{l=1}^{m_k} \sigma^{[\boldsymbol{\alpha}]}_{\boldsymbol{j}}(k,l) \partial^{\boldsymbol{i}_{k,l}}_{\boldsymbol{x}} g(\boldsymbol{c}_k) = \mathcal{S}_{\boldsymbol{\alpha}}[\partial^{2\boldsymbol{j}+\boldsymbol{1}}_{\boldsymbol{x}} g](\boldsymbol{1}) \qquad (4.7)$$

is correct for all polynomials in a given basis of cardinality $m^\star$. In place of interpolation, followed by quadrature, we reduce the problem at hand to the approximation of derivatives by finite differences. We will pursue this further in the sequel.

To illustrate this in $d = 2$, consider $N = 1$ and three configurations of quadrature points $\boldsymbol{c}_k$, all with multiplicity $m_k \equiv 1$:



(a) (b) (c)

Thus, for (a) we have $s = 8$ and the quadrature points are $(\pm1,\pm1)$, $(\pm1,0)$ and $(0,\pm1)$. For both (b) and (c) there are $s = 12$ points, namely $(\pm1,\pm1)$, $(\pm r,\pm2r)$ and $(\pm2r,\pm r)$ for (b) and $(\pm1,\pm1)$, $(\pm1,\pm r)$ and $(\pm r,\pm1)$ for (c). Here $r \in (0,\frac{1}{2})$ is a parameter: we have used $r = \frac{1}{3}$ in our examples.

Let us consider (a) first, explaining our procedure in some detail. The interpolation conditions (4.5) reduce to

$$\partial_x\partial_y\psi(\boldsymbol{c}_k) = \partial_x\partial_y f(\boldsymbol{c}_k), \qquad k = 1,\ldots,8.$$

In other words, letting $\Psi = \psi_{xy}$ and $F = f_{xy}$, we reduce the problem to the bivariate Lagrangian interpolation

$$\Psi(\boldsymbol{c}_k) = F(\boldsymbol{c}_k), \qquad k = 1, \ldots, 8.$$

We have eight degrees of freedom, hence we take

$$\Psi(x,y) = a_1 + a_2 x + a_3 y + a_4 x^2 + a_5 xy + a_6 y^2 + a_7 x^y + a_8 xy^2.$$

Lengthy, yet straightforward, computer algebra results in the method

$$\mathcal{Q}^{[0,0]}_{m,n} = \mathcal{A}^{[0,0]}_{m,n},$$

$$\mathcal{Q}^{[0,1]}_{m,n} = \mathcal{A}^{[0,1]}_{m,n} + \frac{2(-1)^{m+n}}{\pi^6 m^2 (n-\frac{1}{2})^4} \begin{array}{ccc} -1 & 0 & +1 \\ +2 & & -2 \\ -1 & 0 & +1 \end{array} f_{xy},$$

$$\mathcal{Q}^{[1,0]}_{m,n} = \mathcal{A}^{[1,0]}_{m,n} + \frac{2(-1)^{m+n}}{\pi^6 (m-\frac{1}{2})^4 n^2} \begin{array}{ccc} -1 & -2 & +1 \\ 0 & & 0 \\ +1 & +2 & -1 \end{array} f_{xy},$$

$$\mathcal{Q}^{[1,1]}_{m,n} = \mathcal{A}^{[1,1]}_{m,n} - \frac{2(-1)^{m+n}}{\pi^6 (m-\frac{1}{2})^2 (n-\frac{1}{2})^4} \begin{array}{ccc} +1 & 0 & +1 \\ -2 & & -2 \\ +1 & 0 & +1 \end{array} f_{xy}$$

$$- \frac{2(-1)^{m+n}}{(m-\frac{1}{2})^4 (n-\frac{1}{2})^2} \begin{array}{ccc} +1 & -2 & +1 \\ 0 & & 0 \\ +1 & -2 & +1 \end{array} f_{xy}.$$

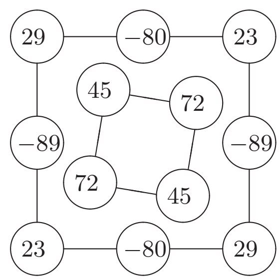
Likewise, for (b) and (c) we have twelve degrees of freedom and in both cases choose

$$\Psi(x,y) = a_1 + a_2x + a_3y + a_4x^2 + a_5xy + a_6y^2 + a_7x^3 + a_8x^2y + a_9xy^2 + a_{10}y^3 + a_{11}x^3 + a_{12}xy^3.$$

Note that the underlying interpolation problems have a unique solution – this was also the case for (a) but not if the inner square in the stencil corresponding to (b) is not slanted.

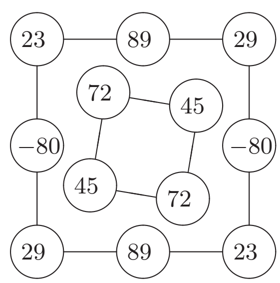
The outcome are the methods

$$\mathcal{Q}^{[0,0]}_{m,n} = \mathcal{A}^{[0,0]}_{m,n} + \tfrac{18}{13}\frac{(-1)^{m+n}}{\pi^6 m^2 n^4}$$



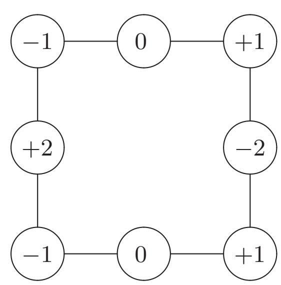
f_{xy}

$$-\tfrac{18}{13}\frac{(-1)^{m+n}}{\pi^6 m^4 n^2}$$



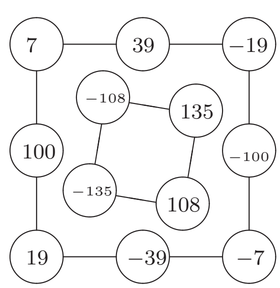
$f_{xy},$

$$\mathcal{Q}^{[0,1]}_{m,n} = \mathcal{A}^{[0,1]}_{m,n} + \frac{2(-1)^{m+n}}{\pi^6 m^2 (n-\frac{1}{2})^4}$$

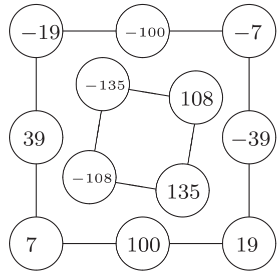


f_{xy}

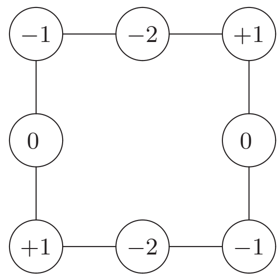
$$-\tfrac{6}{41}\frac{(-1)^{m+n}}{\pi^6 m^4 (n-\frac{1}{2})^2}$$



$f_{xy},$

$$\mathcal{Q}^{[1,0]}_{m,n} = \mathcal{A}^{[1,0]}_{m,n} - \tfrac{6}{41}\frac{(-1)^{m+n}}{\pi^6(m-\frac{1}{2})^2 n^4}$$


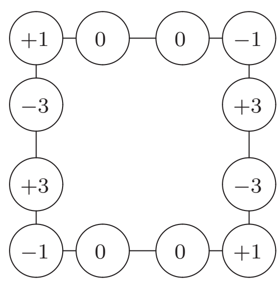
$$f_{xy}$$

$$+\frac{2(-1)^{m+n}}{\pi^6(m-\frac{1}{2})^4 n^2}$$


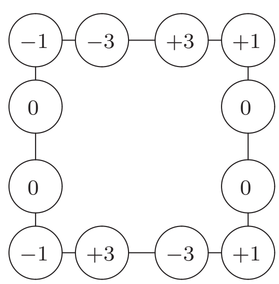
$$f_{xy},$$

$\mathcal{Q}^{[1,1]}_{m,n} =$ the same as in case (a).

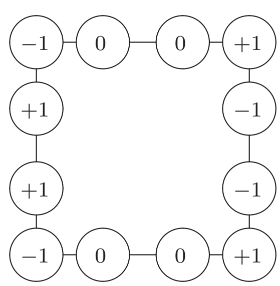
Finally, in case (c) we have

$$\mathcal{Q}^{[0,0]}_{m,n} = \mathcal{A}^{[0,0]}_{m,n} + \frac{4(-1)^{m+n}}{\pi^6 m^2 n^4}$$


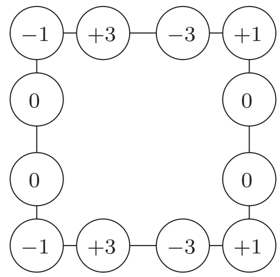
$$f_{xy}$$

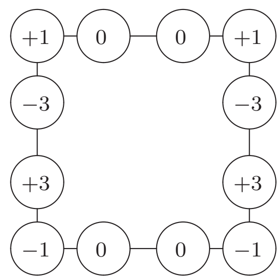
$$+\frac{4(-1)^{m+n}}{\pi^6 m^4 n^2}$$


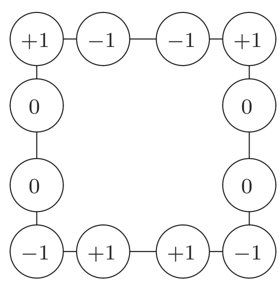
$$f_{xy},$$

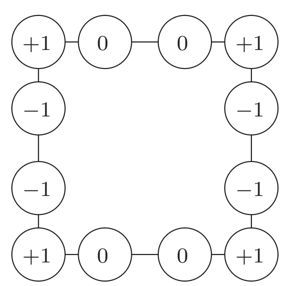
$$\mathcal{Q}^{[0,1]}_{m,n} = \mathcal{A}^{[0,1]}_{m,n} + \tfrac{4}{9}\frac{(-1)^{m+n}}{\pi^6 m^2 (n-\frac{1}{2})^4}$$


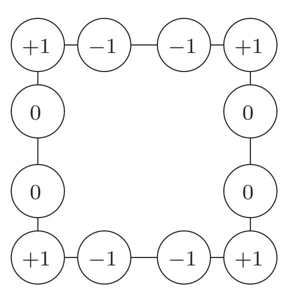
$$f_{xy}$$

$$+\ \tfrac{4}{3}\frac{(-1)^{m+n}}{\pi^6 m^4 (n-\frac{1}{2})^2}$$  f_{xy},

$$\mathcal{Q}^{[1,0]}_{m,n} = \mathcal{A}^{[1,0]}_{m,n} + \tfrac{4}{3}\frac{(-1)^{m+n}}{\pi^6 (m-\frac{1}{2})^2 n^4}$$  f_{xy}

$$+\ \tfrac{4}{9}\frac{(-1)^{m+n}}{\pi^6 (m-\frac{1}{2})^4 n^2}$$  f_{xy},

$$\mathcal{Q}^{[1,1]}_{m,n} = \mathcal{A}^{[1,1]}_{m,n} + \tfrac{4}{9}\frac{(-1)^{m+n}}{\pi^6 (m-\frac{1}{2})^2 (n-\frac{1}{2})^4}$$  f_{xy}

$$-\ \tfrac{4}{9}\frac{(-1)^{m+n}}{\pi^6 (m-\frac{1}{2})^4 (n-\frac{1}{2})^2}$$  f_{xy}.

$\boldsymbol{n}$	$\boldsymbol{\alpha}$	Method (a)	Method (b)	Method (c)
$[1,1]$	$[0,0]$	1.2387_{-01}	1.4931_{-02}	5.4150_{-03}
	$[1,0]$	8.4921_{-02}	9.2728_{-03}	7.4304_{-02}
	$[0,1]$	3.8306_{-01}	3.2903_{-02}	1.3309_{-01}
	$[1,1]$	1.1586_{+00}	1.1586_{+00}	1.3190_{+00}
$[2,3]$	$[0,0]$	6.4873_{-04}	1.5634_{-03}	1.2678_{-04}
	$[1,0]$	8.7572_{-04}	6.8660_{-04}	5.3409_{-04}
	$[0,1]$	1.1945_{-03}	6.2396_{-04}	4.8653_{-04}
	$[1,1]$	1.5549_{-03}	1.5549_{-03}	1.5203_{-03}
$[7,4]$	$[0,0]$	1.1929_{-05}	1.7825_{-05}	3.3349_{-06}
	$[1,0]$	1.3234_{-05}	1.2591_{-05}	1.1881_{-05}
	$[0,1]$	1.7236_{-05}	7.6216_{-06}	5.4031_{-06}
	$[1,1]$	1.8892_{-05}	1.8892_{-05}	1.8530_{-05}
$[10,10]$	$[0,0]$	1.7659_{-07}	3.7784_{-08}	7.7300_{-08}
	$[1,0]$	1.5408_{-07}	1.3313_{-07}	1.1536_{-07}
	$[0,1]$	2.2221_{-07}	1.0698_{-07}	8.0162_{-08}
	$[1,1]$	1.8429_{-07}	1.8429_{-07}	1.8088_{-07}

Table 2: Absolute value of the errors committed by the Filon-type methods (a), (b) and (c), four different $\boldsymbol{n}$s and $f(x,y)=\mathrm{e}^{x-2y}$.

With enough persistence, it is possible to derive this kind of schemes for larger number of quadrature points and for higher derivatives. Yet, it is quite clear that this brute-force approach rapidly leads to unacceptable complexity, to say nothing of the case $d \geq 3$. Moreover, as apparent from Table 2 and comparison with Table 1, the three above schemes represent fairly modest improvement in comparison with the basic asymptotic method $\mathcal{A}_{\boldsymbol{n},1}^{[\boldsymbol{\alpha}]}$, hence the imperative of using more interpolation points is much more than just a matter of idle quest for generality. This motivates the work of the next subsection, where, building upon the interpretation (4.6), we construct Filon-type methods for large number of points, higher derivatives and arbitrary dimensions in a structured manner.

4.3 Extended Filon methods on a tartan grid

The methods (a)–(c) from the last subsection, while delivering but a minor improvement in comparison with the asymptotic method $\mathcal{A}_{\boldsymbol{n},1}^{[\boldsymbol{\alpha}]}$, are fairly cumbersome to construct. Had we followed along the same path and attempted to design more effective methods, whether using higher derivatives or more points or both, this would have resulted in unacceptable complexity – and all this just in two variables and only for expansion terms of grade d.

In the current subsection we develop an alternative approach which cuts across all the problems of the last paragraph. Thus, it allows fairly transparent and automatic construction of methods with arbitrary number of derivatives and large number of points, for all $d \geq 1$ and (although we defer that issue to the next subsection) relevant to terms of all grades.

Our first ingredient is the interpretation (4.6) of a Filon-type method as "an asymptotic method plus an approximation to the next expansion term". This we generalise in the following manner. Suppose that we have evaluated the function f or its derivatives in some grid $\boldsymbol{R}$ in $[-1,1]^d$ – note that we do not assume that the same derivatives are evaluated at each point of the grid. We denote the set of all these function and derivative values by $\mathcal{F}$ and suppose that $\mathcal{F}$ contains all derivative values necessary for the construction of the asymptotic method $\mathcal{A}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},N}$. An *extended Filon method* is

$$\mathcal{Q}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},N,M} = \mathcal{A}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},N} + (-1)^{|\boldsymbol{n}|+|\boldsymbol{\alpha}|} \sum_{m=N}^{N+M-1} \frac{(-1)^m}{\pi^{2(m+d)}} \sum_{|\boldsymbol{j}|=m} \frac{\mathcal{E}^{[\boldsymbol{\alpha}]}_{\boldsymbol{j}}[f]}{\mu^{[\alpha_1]\,2j_1+2}_{n_1} \cdots \mu^{[\alpha_d]\,2j_d+2}_{n_d}}, \tag{4.8}$$

where (compare with (4.7))

$$\mathcal{E}^{[\boldsymbol{\alpha}]}_{\boldsymbol{j}}[f] = \sum_{\boldsymbol{c}\in\boldsymbol{R}} \sum_{\boldsymbol{i}\in\Pi(\boldsymbol{c})} \sigma^{[\boldsymbol{\alpha}]}_{\boldsymbol{j}}(k,l)\partial^{\boldsymbol{i}}_{\boldsymbol{x}} f(\boldsymbol{c}) \approx \mathcal{S}_{\boldsymbol{\alpha}}[\partial^{2\boldsymbol{j}+\boldsymbol{1}}_{\boldsymbol{x}} f](\boldsymbol{1}), \qquad N \le |\boldsymbol{j}| \le N+M-1, \tag{4.9}$$

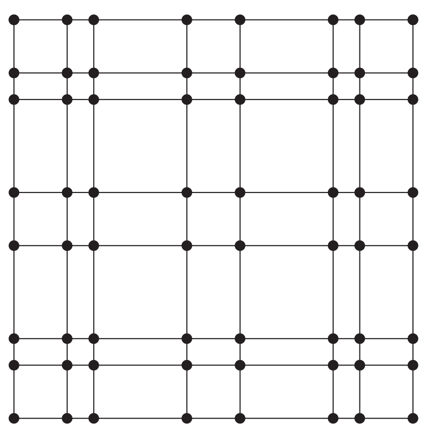
and $\Pi(\boldsymbol{c})$ is the set of all the derivatives of f evaluated at $\boldsymbol{c} \in \boldsymbol{R}$ – in other words,

$$\boldsymbol{i} \in \Pi(\boldsymbol{c}) \qquad \Rightarrow \qquad \partial^{\boldsymbol{i}}_{\boldsymbol{x}} f(\boldsymbol{c}) \in \mathcal{F}.$$

Our next ingredient is the sort of grid $\boldsymbol{R}$ that we find particularly advantageous in structured use of Cartesian products in $[-1,1]^d$: a *tartan grid*. Let the points $r_1 < r_2 < \cdots < r_\nu = 1$ be given, where $r_1 > 0$. Then

$$\boldsymbol{R} = \{(r_{i_1}(-1)^{e_1}, r_{i_2}(-1)^{e_2}, \ldots, r_{i_d}(-1)^{e_d}) \,:\, \boldsymbol{e} \in \mathbb{Z}_2^d,\ i_1,\ldots,i_d \in \{1,2,\ldots,\nu\}\}. \tag{4.10}$$

For example (in this subsection the narrative applies to general $d \ge 1$ but examples, for obvious reasons, are for $d = 2$), letting $\nu = 4$, we might have the grid



We commence our discussion from the case $N = 1$ and $\Pi(\boldsymbol{c}) = \boldsymbol{1}$ for all $\boldsymbol{c} \in \boldsymbol{R}$: in other words, we evaluate just the cross-derivative $\partial^{\boldsymbol{1}}_{\boldsymbol{x}} f$ at every grid point.

Proposition 5 *Given $s \in \{0, 1, \ldots, \nu\}$, there exist coefficients $a_k^{[0,s]}, a_k^{[1,s]}$ such that*

$$\sum_{k=1}^{\nu} a_k^{[0,s]} \sinh r_k\theta = \theta^{2s} \sinh\theta + \mathcal{O}\big(\theta^{2\nu+1}\big)\,, \tag{4.11}$$

$$\sum_{k=1}^{\nu} a_k^{[1,s]} \cosh r_k\theta = \theta^{2s} \cosh\theta + \mathcal{O}\big(\theta^{2\nu}\big)\,. \tag{4.12}$$

Proof We prove our assertion just for (4.11), since the proof of (4.12) is identical. Comparing the Taylor expansions

$$\sum_{k=1}^{\nu} a_k^{[0,s]} \sinh r_k\theta = \sum_{m=0}^{\infty} \frac{1}{(2m+1)!} \left[\sum_{k=1}^{\nu} a_k^{[0,s]} r_k^{2m+1}\right] \theta^{2m+1},$$

$$\theta^{2s} \sinh\theta = \sum_{m=s}^{\infty} \frac{1}{(2m-2s+1)!} \theta^{2m+1},$$

we deduce that (4.11) is equivalent to the Vandermonde linear algebraic system

$$\sum_{k=1}^{\nu} a_k^{[0,s]} r_k^{2m+1} = \begin{cases} 0, & m = 0, \ldots, s-1, \\ \frac{(2m+1)!}{(2m-2s+1)!}, & m = s, \ldots, \nu-1. \end{cases}$$

The system being nonsingular, the assertion of the proposition follows. □

Note that we trivially have $a_k^{[i,0]} = 0$ for $k = 1, \ldots, \nu-1$, $i = 0, 1$ and $a_\nu^{[i,0]} = 1$. Moreover, $\boldsymbol{a}^{[i,s]} = \mathbf{0}$ for $s \geq \nu$.

Theorem 6 *The sum*

$$\sum_{k_1=1}^{\nu} \sum_{k_2=1}^{\nu} \cdots \sum_{k_d=1}^{\nu} \left(\prod_{j=1}^{d} a_{k_j}^{[\alpha_j, s_j]}\right) \mathcal{S}_{\boldsymbol{\alpha}}[\partial_{\boldsymbol{x}}^{\mathbf{1}} f](r_{k_1}, r_{k_2}, \ldots, r_{k_d}) \tag{4.13}$$

coincides with $\mathcal{S}_{\boldsymbol{\alpha}}[\partial_{\boldsymbol{x}}^{2\boldsymbol{s}+\mathbf{1}} f](\mathbf{1})$ for all functions f which are polynomials of degree $2\nu+1$ in all their variables.

Proof We adopt the language of *shift* and *differential* operators E_x and ∂_x respectively and recall that for an analytic function f it is formally true that

$$f(y_1, y_2, \ldots, y_d) = E_{x_1}^{y_1} E_{x_2}^{y_2} \cdots E_{x_d}^{y_d} f(\mathbf{0}) = \mathrm{e}^{y_1\partial_{x_1}} \mathrm{e}^{y_2\partial_{x_2}} \cdots \mathrm{e}^{y_d\partial_{x_d}} f(\mathbf{0}).$$

Since

$$\mathcal{S}_{\boldsymbol{\alpha}}[\partial_{\boldsymbol{x}}^{2\boldsymbol{s}+\mathbf{1}} f](\boldsymbol{y}) = \sum_{\boldsymbol{e}\in\mathbb{Z}_2^d} (-1)^{|\boldsymbol{e}|+\boldsymbol{e}^\top\boldsymbol{\alpha}} \partial_{x_1}^{2s_1} \cdots \partial_{x_d}^{2s_d} E_{x_1}^{(-1)^{e_1} y_1} \cdots E_{x_d}^{(-1)^{e_d} y_d} g(\mathbf{0}),$$

where $g(\boldsymbol{x}) = \partial_{\boldsymbol{x}}^{\mathbf{1}} f(\boldsymbol{x})$, it is true that

$$\sum_{k_1=1}^{\nu}\sum_{k_2=1}^{\nu}\cdots\sum_{k_d=1}^{\nu}\left(\prod_{j=1}^{d} a_{k_j}^{[\alpha_j,s_j]}\right)\mathcal{S}_{\boldsymbol{\alpha}}[\partial_{\boldsymbol{x}}^{\mathbf{2s+1}} f](r_{k_1}, r_{k_2}, \ldots, r_{k_d})$$

$$= \sum_{k_1=1}^{\nu}\sum_{k_2=1}^{\nu}\cdots\sum_{k_d=1}^{\nu}\left(\prod_{j=1}^{d} a_{k_j}^{[\alpha_j,s_j]}\right)\sum_{\boldsymbol{e}\in\mathbb{Z}_2^d}(-1)^{|\boldsymbol{e}|+\boldsymbol{e}^\top\boldsymbol{\alpha}}\partial_{x_1}^{2s_1}\partial_{x_2}^{2s_2}\cdots\partial_{x_d}^{2s_d}$$

$$\times E_{x_1}^{(-1)^{e_1}r_{k_1}} E_{x_2}^{(-1)^{e_2}r_{k_2}}\cdots E_{x_d}^{(-1)^{e_d}r_{k_d}} g(\mathbf{0}).$$

Note, however, that, by easy induction,

$$\sum_{\boldsymbol{e}\in\mathbb{Z}_2^d}(-1)^{|\boldsymbol{e}|+\boldsymbol{e}^\top\boldsymbol{\alpha}}\mathrm{e}^{(-1)^{e_1}r_{k_1}\partial_{x_1}+\cdots+(-1)^{e_d}r_{k_d}\partial_{x_d}}$$

$$= \sum_{\boldsymbol{e}\in\mathbb{Z}_2^{d-1}}(-1)^{|\boldsymbol{e}|+\boldsymbol{e}^\top\boldsymbol{\alpha}}\mathrm{e}^{(-1)^{e_1}r_{k_1}\partial_{x_1}+\cdots+(-1)^{e_{d-1}}r_{k_{d-1}}\partial_{x_{d-1}}}[\mathrm{e}^{r_{k_d}\partial_{x_d}} - (-1)^{\alpha_d}\mathrm{e}^{-r_{k_d}\partial_{x_d}}]$$

$$\cdots = \prod_{j=1}^{d}[\mathrm{e}^{r_{k_j}\partial_{x_j}} - (-1)^{\alpha_j}\mathrm{e}^{-r_{k_j}\partial_{x_j}}].$$

Consequently,

$$\sum_{k_1=1}^{\nu}\sum_{k_2=1}^{\nu}\cdots\sum_{k_d=1}^{\nu}\left(\prod_{j=1}^{d} a_{k_j}^{[\alpha_j,s_j]}\right)\mathcal{S}_{\boldsymbol{\alpha}}[\partial_{\boldsymbol{x}}^{\mathbf{1}} f](r_{k_1}, r_{k_2}, \ldots, r_{k_d})$$

$$= \sum_{k_1=1}^{\nu}\sum_{k_2=1}^{\nu}\cdots\sum_{k_d=1}^{\nu}\left(\prod_{j=1}^{d} a_{k_j}^{[\alpha_j,s_j]}\partial_{x_j}^{2s_j}\right)\prod_{j=1}^{d}[\mathrm{e}^{r_{k_j}\partial_{x_j}} - (-1)^{\alpha_j}\mathrm{e}^{-r_{k_j}\partial_{x_j}}]g(\mathbf{0})$$

$$= \prod_{j=1}^{d}\left\{\partial_{x_j}^{2s_j}\sum_{k=1}^{\nu} a_k^{[\alpha_j,s_j]}[\mathrm{e}^{r_k\partial_{x_j}} - (-1)^{\alpha_j}\mathrm{e}^{-r_k\partial_{x_j}}]\right\} g(\mathbf{0})$$

Note further that for $\alpha_j = 0$

$$\sum_{k=1}^{\nu} a_k^{[\alpha_j,s_j]}[\mathrm{e}^{r_k\partial_{x_j}} - (-1)^{\alpha_j}\mathrm{e}^{-r_k\partial_{x_j}}] = 2\sum_{k=1}^{\nu} a_k^{[\alpha_j,s_j]}\sinh(r_k\partial_{x_j}),$$

while $\alpha_j = 1$ yields

$$\sum_{k=1}^{\nu} a_k^{[\alpha_j,s_j]}[\mathrm{e}^{r_k\partial_{x_j}} - (-1)^{\alpha_j}\mathrm{e}^{-r_k\partial_{x_j}}] = 2\sum_{k=1}^{\nu} a_k^{[\alpha_j,s_j]}\cosh(r_k\partial_{x_j}).$$

Likewise,

$$\mathcal{S}_{\boldsymbol{\alpha}}[\partial_{\boldsymbol{x}}^{\mathbf{2s+1}} f](\mathbf{1}) = \prod_{j-1}^{d}\partial_{x_j}^{2s_j}[\mathrm{e}^{\partial_{x_j}} - (-1)^{\alpha_j}\mathrm{e}^{-\partial_{x_j}}]g(\mathbf{0})$$

and again we can replace the term in square brackets with either $2\sinh\partial_{x_j}$ or $2\cosh\partial_{x_j}$, depending on α_j being 0 or 1, respectively. Comparison of the two expressions, in tandem with (4.11), (4.12) and $g=\partial_{x_1}\cdots\partial_{x_d}f$, prove the theorem. $\square$

Our first concrete example of an extended Filon method is

$$\mathcal{Q}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},1,2,\nu}=\mathcal{A}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},1}-\frac{(-1)^{|\boldsymbol{n}|+|\boldsymbol{\alpha}|}}{\pi^{2(d+1)}}\sum_{|\boldsymbol{j}|=1}\frac{1}{\mu^{[\alpha_1]\,2j_1+2}_{n_1}\cdots\mu^{[\alpha_d]\,2j_d+2}_{n_d}}\times\sum_{k_1=1}^{\nu}\cdots\sum_{k_d=1}^{\nu}\left(\prod_{j=1}^{d}a^{[\alpha_j,j_k]}_{k_j}\right)\mathcal{S}_{\boldsymbol{\alpha}}[\partial^{\boldsymbol{1}}_{\boldsymbol{x}}f](r_{k_1},\ldots,r_{k_d}). \tag{4.14}$$

In the same vain we let

$$\mathcal{Q}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},1,3,\nu}=\mathcal{Q}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},1,2,\nu}+\frac{(-1)^{|\boldsymbol{n}|+|\boldsymbol{\alpha}|}}{\pi^{2(d+2)}}\sum_{|\boldsymbol{j}|=2}\frac{1}{\mu^{[\alpha_1]\,2j_1+2}_{n_1}\cdots\mu^{[\alpha_d]\,2j_d+2}_{n_d}}\times\sum_{k_1=1}^{\nu}\cdots\sum_{k_d=1}^{\nu}\left(\prod_{j=1}^{d}a^{[\alpha_j,j_k]}_{k_j}\right)\mathcal{S}_{\boldsymbol{\alpha}}[\partial^{\boldsymbol{1}}_{\boldsymbol{x}}f](r_{k_1},\ldots,r_{k_d}) \tag{4.15}$$

and so on, up to $\mathcal{Q}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},1,\nu,\nu}$. In general, $\mathcal{Q}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},N,M,\nu}$ uses the first N odd derivatives on the tartan grid to approximate the next $M-N$ odd derivatives at the vertices. In other words, it updates the asymptotic method $\mathcal{A}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},N}$ with a finite-difference of the remaining terms in $\mathcal{A}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},M}$.

It is important to quantify the computational cost and suitable means of implementation of extended Filon methods like (4.14) and (4.15):

1. We commence by computing $\partial_{x_1}\partial_{x_2}\cdots\partial_{x_d}f$ on the tartan grid: altogether, $(2\nu)^d$ derivative evaluations.

2. Next, we precompute quantities of the form

$$\sigma^{[\boldsymbol{\alpha}]}_{\boldsymbol{j}}=\frac{(-1)^{m+|\boldsymbol{\alpha}|}}{\pi^{2m+2d}}\mathcal{S}_{\boldsymbol{\alpha}}[\partial^{2\boldsymbol{j}+\boldsymbol{1}}_{\boldsymbol{x}}f](\boldsymbol{1}),\qquad m=0,\ldots,N-1,\quad \boldsymbol{\alpha}\in\mathbb{Z}_2^d$$

   and

$$\sigma^{[\boldsymbol{\alpha}]}_{\boldsymbol{j}}=\frac{(-1)^{m+|\boldsymbol{\alpha}|}}{\pi^{2m+2d}}\sum_{k_1=1}^{\nu}\cdots\sum_{k_d=1}^{\nu}\left(\prod_{j=1}^{d}a^{[\alpha_j,j_k]}_{k_j}\right)\mathcal{S}_{\boldsymbol{\alpha}}[\partial^{\boldsymbol{1}}_{\boldsymbol{x}}f](r_{k_1},\ldots,r_{k_d})$$

   for $m=N,\ldots,M-1$ and $\boldsymbol{\alpha}\in\mathbb{Z}_2^d$.

3. Finally, for every $\boldsymbol{n}\in\mathbb{N}^d$ of interest, we form the linear combination

$$\mathcal{Q}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},N,M,\nu}=(-1)^{|\boldsymbol{n}|}\sum_{m=0}^{M}\sum_{|\boldsymbol{j}|=m}\frac{\sigma^{[\boldsymbol{\alpha}]}_{\boldsymbol{j}}}{\mu^{[\alpha_1]\,2j_1+2}_{n_1}\cdots\mu^{[\alpha_d]\,2j_d+2}_{n_d}}.$$

$\boldsymbol{n}$	$\boldsymbol{\alpha}$	$\mathcal{Q}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},1,2,3}$	$\mathcal{Q}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},1,3,3}$	$\mathcal{Q}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},1,2,4}$	$\mathcal{Q}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},2,3,3}$	$\tilde{\mathcal{Q}}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},2,3,3}$
$[1,1]$	$[0,0]$	5.0405_{-02}	4.7641_{-03}	5.3270_{-02}	4.2553_{-03}	2.0422_{-02}
	$[1,0]$	5.6043_{-01}	1.4023_{-01}	5.8154_{-01}	2.2828_{-01}	3.1139_{-01}
	$[0,1]$	1.3929_{+00}	1.4166_{-01}	1.5393_{+00}	2.1693_{+00}	2.1694_{+00}
	$[1,1]$	9.0370_{+00}	3.2836_{+00}	9.8311_{+00}	1.4573_{+01}	1.4566_{+01}
$[2,3]$	$[0,0]$	2.5611_{-04}	3.7868_{-06}	3.4693_{-05}	4.8262_{-06}	1.1911_{-06}
	$[1,0]$	9.9682_{-05}	7.1106_{-06}	1.2863_{-04}	6.6283_{-06}	6.0393_{-06}
	$[0,1]$	2.3085_{-04}	2.7402_{-05}	8.2995_{-05}	5.0529_{-07}	3.5428_{-07}
	$[1,1]$	1.2645_{-04}	6.1027_{-06}	2.7600_{-04}	7.8830_{-06}	7.8300_{-06}
$[7,4]$	$[0,0]$	6.3459_{-08}	1.5005_{-07}	2.8844_{-07}	7.9156_{-08}	1.1813_{-10}
	$[1,0]$	9.1392_{-08}	2.3913_{-07}	4.4550_{-07}	1.2014_{-07}	5.1403_{-11}
	$[0,1]$	6.7342_{-07}	9.3961_{-07}	5.7105_{-07}	3.7894_{-08}	3.7881_{-08}
	$[1,1]$	1.0304_{-06}	1.4448_{-06}	8.8030_{-07}	5.7017_{-08}	5.7370_{-08}
$[10,10]$	$[0,0]$	3.3656_{-09}	1.9034_{-08}	1.6589_{-08}	1.8096_{-09}	4.3265_{-11}
	$[1,0]$	1.5307_{-08}	4.9295_{-08}	4.1323_{-08}	1.7826_{-09}	2.7506_{-11}
	$[0,1]$	5.7149_{-08}	7.4508_{-08}	1.5752_{-08}	1.2754_{-09}	2.2044_{-10}
	$[1,1]$	1.0861_{-07}	1.4674_{-07}	4.2167_{-08}	6.6095_{-10}	6.6534_{-10}

Table 3: Absolute value of the errors committed by extended Filon methods for five different $\boldsymbol{n}$s and $f(x,y)=\mathrm{e}^{x-2y}$.

The overall cost is *linear* in the number of coefficients $\hat{f}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n}}$ that we wish to approximate in this manner.

Note, additionally, that in the special case $N=1, M=2$ we deduce from $\boldsymbol{a}^{[\alpha,0]}=\mathbf{0}$ that only points along the perimeter of the grid feature with nonzero coefficients. Thus, in place of $(2\nu)^d$ function evaluations, it suffices to compute the derivative of f at just $(2\nu)^d-[2(\nu-1)]^d\approx d2^d\nu^{d-1}$ points at the intersection of the boundary with the tartan grid.

To flesh out numbers, let $\nu=3$ and

$$r_1=\frac{\sqrt{495-66\sqrt{15}}}{33},\qquad r_2=\frac{\sqrt{495+66\sqrt{15}}}{33},\qquad r_3=1$$

(the reason for this choice will be apparent in the next section). Easy calculation confirms that

$$\begin{aligned}
\boldsymbol{a}^{[0,1]}&=[\,-\tfrac{99}{10}\tfrac{100-49\sqrt{15}}{\sqrt{495-66\sqrt{15}}}\quad -\tfrac{99}{10}\tfrac{100+49\sqrt{15}}{\sqrt{495+66\sqrt{15}}}\quad 60\,],\\
\boldsymbol{a}^{[1,1]}&=[\,-21+\tfrac{23}{2}\sqrt{15}\quad -21-\tfrac{23}{2}\sqrt{15}\quad 42\,]\\
\boldsymbol{a}^{[0,2]}&=[\,-\tfrac{3267}{2}\tfrac{5-3\sqrt{15}}{\sqrt{495-66\sqrt{15}}}\quad -\tfrac{3267}{2}\tfrac{5+3\sqrt{15}}{\sqrt{495+66\sqrt{15}}}\quad 495\,]\\
\boldsymbol{a}^{[1,2]}&=[\,-\tfrac{99}{2}+\tfrac{297}{10}\sqrt{15}\quad -\tfrac{99}{2}-\tfrac{297}{10}\sqrt{15}\quad 99\,].
\end{aligned}$$

It is apparent from the three leftmost columns in Table 3 that, while the performance for $\bar{n}\leq 2$ is still unacceptably poor, the performance of extended Filon definitely leads to smaller error for larger $\bar{n}$s.

Another, most unwelcome, observation is that the errors in $\mathcal{Q}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},1,2,3}$ and $\mathcal{Q}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n},1,3,3}$ are roughly similar, at least for the reported values of $\boldsymbol{n}$. A probable reason is that the magnitude of the coefficients of $\boldsymbol{a}^{[\alpha,j]}$ increases fairly rapidly with j. Thus, methods really 'take off' only for fairly large $\bar{n}$ – for example, the errors of $\mathcal{Q}^{[0,0]}_{[20,20],1,3,3}$ and $\mathcal{Q}^{[0,0]}_{[20,20],1,2,4}$ are 1.1867_{-09} and 1.2941_{-13} – the latter is fairly respectable.

Indeed, a significant downside of our approach is that the approximation of derivatives is a notoriously ill-conditioned problem. An effective design of extended Filon methods for significantly larger values of ν might well abandon altogether the goal of maximising order of approximation in (4.11) and (4.12). A more suitable approach is probably to choose least-norm vectors $\boldsymbol{a}^{[\alpha,j]}$ consistent with lower order, or perhaps just to give up on extended Filon, reconcile ourselves to compute higher derivatives and use an asymptotic method. We do not pursue this issue further in this paper but might return to it in future publications.

Extended Filon methods (4.14) and (4.15) are both based on computing only the cross-derivative $\partial_{x_1}\cdots\partial_{x_d}f$ on the tartan grid. An obvious – yet unnecessary – next step is to compute there *both* $\partial_{x_1}\cdots\partial_{x_d}f$ and $\partial_{x_1}\cdots\partial_{x_{i-1}}\partial^3_{x_i}\partial_{x_{i+1}}\cdots\partial_{x_d}f$ for all $i=1,\ldots,d$. This, however is an overkill and represents poor use of computational resources.

Recall from the asymptotic expansion (3.6) that asymptotic order is determined exclusively by derivatives at the vertices. Thus, the sole purpose of using derivative values elsewhere in the cube is to approximate higher derivatives at the vertices. In principle, thus, we could have computed intermediate derivatives just at the vertices. Our approach strikes a middle course, since it leads to far simpler and more transparent expressions for general d: We compute

1. The cross-derivative $\partial^{\boldsymbol{1}}_{\boldsymbol{x}}f$ on the tartan grid $\boldsymbol{R}$ – this requires $(2\nu)^d$ function evaluations;
2. The next derivative, $\partial^{\boldsymbol{1}+2\boldsymbol{e}_i}_{\boldsymbol{x}}f$, $i=1,\ldots,d$, where $\boldsymbol{e}_i\in\mathbb{R}^d$ is the ith unit vector, on the boundary of $\boldsymbol{R}$: altogether, $2^d[\nu^d-(\nu-1)^d]$ function evaluations;
3. The derivative $\partial^{\boldsymbol{1}+2\boldsymbol{e}_{i_1}+\cdots+2\boldsymbol{e}_{i_r}}_{\boldsymbol{x}}f$, $1\le i_1<\cdots<i_r\le d$, $1\le r\le d$, at the 2^d vertices – altogether $\binom{d}{2}2^d$ values.

Given $s\in\{0,1,\ldots,\nu+1\}$, we consider coefficients $a^{[0,s]}_k$, $a^{[1,s]}_k$, $k=1,\ldots,\nu$, $\tilde{a}^{[0,s]}$ and $\tilde{a}^{[1,s]}$ such that

$$\sum_{k=1}^{\nu} a^{[0,s]}_k \sinh r_k\theta + \tilde{a}^{[0,s]}\theta^2\sinh\theta = \theta^{2s}\sinh\theta + \mathcal{O}\big(\theta^{2\nu+3}\big)\,, \tag{4.16}$$

$$\sum_{k=1}^{\nu} a^{[1,s]}_k \cosh r_k\theta + \tilde{a}^{[1,s]}\theta^2\cosh\theta = \theta^{2s}\cosh\theta + \mathcal{O}\big(\theta^{2\nu+2}\big)\,. \tag{4.17}$$

Note that existence and uniqueness of such coefficients are an open problem. Proceeding like in the proof of Proposition 5, it is easy to show that (4.16), for example, is equivalent to

$$\sum_{k=1}^{\nu} a^{[0,s]}_k r_k^{2m+1} + (2m)(2m+1)\tilde{a}^{[0,s]} = \begin{cases} 0, & m=0,\ldots,s-1,\\ \frac{(2m+1)!}{(2m-2s+1)!}, & m=s,\ldots,\nu. \end{cases}$$

Is this linear system always nonsingular? We do not know. Had we replaced $(2m)(2m+1)$ by $2m$, it would have been easy to prove so by a limiting argument on Vandermonde matrices.

We have confirmed non-singularity for small νs and 'interesting' (in the sense of the next subsection) values of $r_1, \ldots, r_{\nu-1}$ and this is as much as we can say at present juncture of time.

Proceeding similarly to the proof of Theorem 6, we let

$$\mathcal{G}_j^{[i,s]} = \sum_{k=1}^{\nu} a_k^{[i,s]}[\mathrm{e}^{r_k \partial_{x_j}} - (-1)^i \mathrm{e}^{-r_k \partial_{x_j}}] + \tilde{a}^{[i,s]} \partial_{x_j}^2 [\mathrm{e}^{\partial_{x_j}} - (-1)^i \mathrm{e}^{-\partial_{x_j}}],$$

where $i \in \{0, 1\}$ and recall that $g = \partial_{\boldsymbol{x}}^{\mathbf{1}} f$. We now observe that, by virtue of (4.16) and (4.17), it is true that

$$\mathcal{G}_{\boldsymbol{j}}^{[\alpha]} = \prod_{j=1}^{d} \mathcal{G}_j^{[\alpha_j, s_j]}[g](\mathbf{0}) = \mathcal{S}_{\boldsymbol{\alpha}}[\partial_{\boldsymbol{x}}^{2\boldsymbol{s}+\mathbf{1}} f](\mathbf{1}) \tag{4.18}$$

for all polynomials f of degree $2\nu + 4$ in each of their coordinates.

It is important to realise what (4.18) means. We demonstrate this for $d = 2$, noting that the general case is just a matter of more complicated notation. Thus, in two variables

$$\begin{aligned}
\mathcal{G}_{\boldsymbol{j}}^{[\alpha]} = \prod_{j=1}^{2} \mathcal{G}_j^{[\alpha_j, s_j]}[g](\mathbf{0}) &= \sum_{k_1=1}^{\nu} \sum_{k_2=1}^{\nu} a_{k_1}^{[\alpha_1, s_1]} a_{k_2}^{[\alpha_2, s_2]} [\mathrm{e}^{r_{k_1} \partial_{x_1}} - (-1)^{\alpha_1} \mathrm{e}^{-r_{k_1} \partial_{x_1}}] \\
&\quad \times [\mathrm{e}^{r_{k_2} \partial_{x_2}} - (-1)^{\alpha_2} \mathrm{e}^{-r_{k_2} \partial_{x_2}}] \partial_{\boldsymbol{x}}^{[1,1]} f(0,0) \\
&\quad + \tilde{a}^{[\alpha_1, s_1]} \sum_{k_2=1}^{d} a_{k_2}^{[\alpha_2, s_2]} [\mathrm{e}^{\partial_{x_1}} - (-1)^{\alpha_1} \mathrm{e}^{-\partial_{x_1}}] \\
&\quad \times [\mathrm{e}^{r_{k_2} \partial_{x_2}} - (-1)^{\alpha_2} \mathrm{e}^{-r_{k_2} \partial_{x_2}}] \partial_{\boldsymbol{x}}^{[3,1]} f(0,0) \\
&\quad + \tilde{a}^{[\alpha_2, s_2]} \sum_{k_1=1}^{d} a_{k_1}^{[\alpha_1, s_1]} [\mathrm{e}^{\partial_{x_2}} - (-1)^{\alpha_2} \mathrm{e}^{-\partial_{x_2}}] \\
&\quad \times [\mathrm{e}^{r_{k_1} \partial_{x_1}} - (-1)^{\alpha_1} \mathrm{e}^{-r_{k_1} \partial_{x_1}}] \partial_{\boldsymbol{x}}^{[1,3]} f(0,0) \\
&\quad + \tilde{a}^{[\alpha_1, s_1]} \tilde{a}^{[\alpha_2, s_2]} [\mathrm{e}^{\partial_{x_1}} - (-1)^{\alpha_1} \mathrm{e}^{-\partial_{x_1}}][\mathrm{e}^{\partial_{x_2}} - (-1)^{\alpha_2} \mathrm{e}^{-\partial_{x_2}}] \partial_{\boldsymbol{x}}^{[3,3]} f(0,0) \\
&= \sum_{k_1=1}^{\nu} \sum_{k_2=1}^{\nu} a_{k_1}^{[\alpha_1, s_1]} a_{k_2}^{[\alpha_2, s_2]} \mathcal{S}_{\boldsymbol{\alpha}}[f_{x_1 x_2}](r_{k_1}, r_{k_2}) \\
&\quad + \tilde{a}^{[\alpha_1, s_1]} \sum_{k_2=1}^{d} a_{k_2}^{[\alpha_2, s_2]} \mathcal{S}_{\boldsymbol{\alpha}}[f_{x_1 x_1 x_1 x_2}](1, r_{k_2}) \\
&\quad + \tilde{a}^{[\alpha_2, s_2]} \sum_{k_1=1}^{d} a_{k_1}^{[\alpha_1, s_1]} \mathcal{S}_{\boldsymbol{\alpha}}[f_{x_1 x_2 x_2 x_2}](r_{k_1}, 1) \\
&\quad + \tilde{a}^{[\alpha_1, s_1]} \tilde{a}^{[\alpha_2, s_2]} \mathcal{S}_{\boldsymbol{\alpha}}[f_{x_1 x_1 x_1 x_2 x_2 x_2}](1, 1).
\end{aligned}$$

A generalisation for all $d = 3$ is straightforward and it is clear how the derivative information specified above is used.

We now define the extended Filon method $\mathcal{Q}_{\boldsymbol{n},2,M,\nu}^{[\boldsymbol{\alpha}]}$, where $3 \leq M \leq \nu + 1$, as follows: commence from the asymptotic expansion $\mathcal{A}_{\boldsymbol{n},M}^{[\boldsymbol{\alpha}]}$, retain each $\mathcal{S}_{\boldsymbol{\alpha}}[\partial_{\boldsymbol{x}}^{2\boldsymbol{j}+\mathbf{1}} f]$ which we can compute with available data (i.e., $\boldsymbol{j} = \boldsymbol{0}$, $\boldsymbol{j} = \boldsymbol{e}_i$ and $\boldsymbol{j} = \boldsymbol{e}_{i_1} + \boldsymbol{e}_{j_2}$ for $j_1 < j_2$) and replace each remaining $\mathcal{S}_{\boldsymbol{\alpha}}[\partial_{\boldsymbol{x}}^{2\boldsymbol{j}+\boldsymbol{1}} f]$ with $\mathcal{G}_{\boldsymbol{j}}^{[\boldsymbol{\alpha}]}$.

For example, for $d = 2$, letting $M = 3$, we can use exact terms for all choices of $\boldsymbol{j}$, except for $\boldsymbol{j} = [0, 2]$ and $\boldsymbol{j} = [2, 0]$. Moreover,

$$\boldsymbol{a}^{[\alpha,0]} = \boldsymbol{e}_\nu, \quad \tilde{a}^{[\alpha,0]} = 0, \qquad \boldsymbol{a}^{[\alpha,1]} = \boldsymbol{0}, \quad \tilde{a}^{[\alpha,1]} = 1,$$

therefore

$$\mathcal{G}_{0,2}^{[\boldsymbol{\alpha}]} = \sum_{k=1}^{\nu} a_k^{[\alpha_2,2]} \mathcal{S}_{\boldsymbol{\alpha}}[\partial_{x_1}\partial_{x_2} f](1, r_k) + \tilde{a}^{[\alpha_2,2]} \mathcal{S}_{\boldsymbol{\alpha}}[\partial_{x_1}\partial_{x_2}^3 f](1, 1),$$
$$\mathcal{G}_{2,0}^{[\boldsymbol{\alpha}]} = \sum_{k=1}^{\nu} a_k^{[\alpha_1,2]} \mathcal{S}_{\boldsymbol{\alpha}}[\partial_{x_1}\partial_{x_2} f](r_k, 1) + \tilde{a}^{[\alpha_1,2]} \mathcal{S}_{\boldsymbol{\alpha}}[\partial_{x_1}^3\partial_{x_1} f](1, 1).$$

Table 3 displays in its two rightmost columns the error committed by $\mathcal{Q}_{\boldsymbol{n},2,3,3}^{[\boldsymbol{\alpha}]}$ for the function $f(x, y) = \mathrm{e}^{x-2y}$, where we have used at the first instance

$$r_1 = 0.25880489112795273420, \qquad r_2 = 0.71973603716981453919, \qquad r_3 = 1.$$

This choice is designed to maximise, in the spirit of Subsection 5.3, the order of underlying exotic quadrature. Our other choice, denoted $\tilde{\mathcal{Q}}_{\boldsymbol{n},2,3,3}^{[\boldsymbol{\alpha}]}$, corresponds to the fairly arbitrarily chosen $\boldsymbol{r} = [\frac{1}{3}, \frac{2}{3}, 1]$ and it displays considerably better behaviour for large $\bar{n}$. However, it would have led in Section 5 to worse exotic quadrature. In general, the numbers follow the pattern that we have already identified for other extended Filon methods: poor performance for $\bar{n} = 1$, rapid improvement for increasing $\bar{n}$.

5 Exotic quadrature

5.1 The 0-grade coefficient

While extended Filon methods are exceedingly effective for moderately large $\bar{n}$, they are fairly ineffective for small $\bar{n} \geq 1$ and, like asymptotic methods, cannot be used for $\bar{n} = 0$. The main idea of *exotic quadrature* (Iserles & Nørsett 2006*b*) is to reuse the derivatives of f that have been already computed for the implementation of Filon-type methods, to evaluate quadrature formulæ for non-oscillatory integrals. This ultimately leads to non-classical quadrature methods which use both function and derivative values. Although reminiscent of the more familiar *Gauss–Turan methods* (Davis & Rabinowitz 1984), they are of an altogether different kind and present us with novel challenges.

We commence our analysis from the single grade-0 term,

$$\hat{f}_0^{[\boldsymbol{0}]} = \int_{-1}^{1}\int_{-1}^{1}\cdots\int_{-1}^{1} f(\boldsymbol{x})\mathrm{d}x_1\mathrm{d}x_2\cdots\mathrm{d}x_d.$$

It is an easy exercise to prove by repeated integration by parts that

$$d = 1: \qquad \hat{f}_0^{[0]} = f(1) + f(-1) - \int_{-1}^{1} x f_x(x)\mathrm{d}x,$$

$$d=2: \qquad \hat{f}_{\mathbf{0}}^{[0,0]} = [f(1,1)+f(1,-1)+f(-1,1)+f(-1,-1)] \\ - \int_{-1}^{1} x_1[f_{x_1}(x_1,1)+f_{x_1}(x_1,-1)]\mathrm{d}x_1 \\ - \int_{-1}^{1} x_2[f_{x_2}(1,x_2)+f_{x_2}(-1,x_2)]\mathrm{d}x_2 \\ + \int_{-1}^{1}\int_{-1}^{1} x_1x_2 f_{x_1x_2}(x_1,x_2)\mathrm{d}x_1\mathrm{d}x_2.$$

To generalise this construction to all d, we let $\boldsymbol{i}$ be a vector of integers of length m such that $i_1 < i_2 < \cdots < i_m$, $1 \le i_1$ and $i_m \le d$. We denote by $\boldsymbol{\sigma}(\boldsymbol{i})$ the vector of length $d-m$ consisting of the remaining components of $[1,2,\ldots,d]$, in natural order. Given $\boldsymbol{x} \in [-1,1]^d$ and $\boldsymbol{e} \in \mathbb{Z}_2^m$, we let $\boldsymbol{x}_{\boldsymbol{i},\boldsymbol{e}}$ be a vector in $[-1,1]^d$ where

$$(\boldsymbol{x}_{\boldsymbol{i},\boldsymbol{e}})_l = \begin{cases} x_l, & l = i_j \text{ for some } j \in \{1,\ldots,m\}, \\ (-1)^{e_j}, & l = \sigma_j(\boldsymbol{i}) \text{ for some } j \in \{1,\ldots,d-m\}. \end{cases}$$

We extend this in a natural way to the empty sequence $\boldsymbol{i} = \emptyset$. Thus, for example, in $d=4$

$$\boldsymbol{x}_{[1,2,3,4],\emptyset} = [x_1,\ x_2,\ x_3,\ x_4], \qquad \boldsymbol{x}_{[2,4],[e_1,e_2]} = [(-1)^{e_1},\ x_2,\ (-1)^{e_2},\ x_4]$$

and

$$\boldsymbol{x}_{\emptyset,[e_1,e_2,e_3,e_4]} = [(-1)^{e_1},\ (-1)^{e_2},\ (-1)^{e_3},\ (-1)^{e_4}].$$

Finally, we define the operator

$$\mathcal{P}_{\boldsymbol{i}}[f](\boldsymbol{x}) = x_{i_1}\cdots x_{i_m} \sum_{\boldsymbol{e}\in\mathbb{Z}_2^{d-m}} f_{x_{i_1}x_{i_2}\cdots x_{i_m}}(\boldsymbol{x}_{\boldsymbol{i},\boldsymbol{e}}) = x_{i_1}\cdots x_{i_m}\mathcal{S}_{\mathbf{1}}[\partial_{\boldsymbol{x}}^{\mathbf{1}} f](\boldsymbol{x}_{\boldsymbol{i}}).$$

(Note that the operator $\mathcal{S}$ acts only on the $d-m$ coordinates $\boldsymbol{x}_{\boldsymbol{i}}$ complementary to $\boldsymbol{i}$.) Thus,

$$d=1: \qquad \hat{f}_0^{[0]} = \mathcal{P}_\emptyset[f](x) - \int_{-1}^{1}\mathcal{P}_{[1]}[f](x)\mathrm{d}x,$$

$$d=2: \qquad \hat{f}_{\mathbf{0}}^{[0,0]} = \mathcal{P}_\emptyset[f](x_1,x_2) - \int_{-1}^{1}\mathcal{P}_{[1]}[f](x_1,x_2)\mathrm{d}x_1 - \int_{-1}^{1}\mathcal{P}_{[2]}[f](x_1,x_2)\mathrm{d}x_2 \\ + \int_{-1}^{1}\int_{-1}^{1}\mathcal{P}_{[1,2]}[f](x_1,x_2)\mathrm{d}x_1\mathrm{d}x_2.$$

A pattern emerges and it is confirmed in the following proposition.

Proposition 7 *For every $d \ge 1$ it is true that*

$$\hat{f}_{\mathbf{0}}^{[\mathbf{0}]} = \sum_{m=0}^{d}(-1)^m \sum_{\boldsymbol{i}\in U_{d,m}} \int_{-1}^{1}\int_{-1}^{1}\cdots\int_{-1}^{1}\mathcal{P}_{\boldsymbol{i}}[f](\boldsymbol{x})\mathrm{d}x_{i_1}\mathrm{d}x_{i_2}\cdots\mathrm{d}x_{i_m}, \tag{5.1}$$

where $U_{d,m}$ is the set of all strictly monotone sequences of length m from $\{1,2,\ldots,d\}$ and a 0-fold integral is defined as the function itself.

Proof By induction on $d \ge 1$. The assertion is certainly true for $d = 1, 2$. Integrating by parts in x_d, we have

$$\begin{aligned}\hat{f}_{\mathbf{0}}^{[\mathbf{0}]} &= \int_{-1}^{1} \cdots \int_{-1}^{1} [f(x_1, \ldots, x_{d-1}, 1) + f(x_1, \ldots, x_{d-1}, -1)] \mathrm{d}x_1 \cdots \mathrm{d}x_{d-1} \\ &\quad - \int_{-1}^{1} \cdots \int_{-1}^{1} \left[\int_{-1}^{1} x_d f_{x_d}(x_1, \ldots, x_d) \mathrm{d}x_d \right] \mathrm{d}x_1 \cdots \mathrm{d}x_{d-1} \\ &= I_{d-1}[f(\,\cdot\,, \ldots, \,\cdot\,, 1) + f(\,\cdot\,, \ldots, \,\cdot\,, -1)] - I_{d-1} \left[\int_{-1}^{1} x_d f_{x_d}(\,\cdot\,, \ldots, \,\cdot\,, x_d) \mathrm{d}x_d \right],\end{aligned}$$

where $I_m[g] = \hat{g}_{\mathbf{0}}^{[\mathbf{0}]}$ for an m-variate function g.

Let $f_{\pm}(x_1, \ldots, x_{d-1}) = f(x_1, \ldots, x_{d-1}, \pm 1)$. Given $\boldsymbol{i} \in U_{d-1,m}$ it is easy to confirm from the definition of $\mathcal{P}_{\boldsymbol{i}}$ that

$$\mathcal{P}_{\boldsymbol{i}}[f_+] + \mathcal{P}_{\boldsymbol{i}}[f_-] = \mathcal{P}_{\boldsymbol{i}}[f].$$

Therefore, by the induction assumption,

$$I_{d-1}[f_+] + I_{d-1}[f_-] = \sum_{m=0}^{d-1} (-1)^m \sum_{\boldsymbol{i} \in U_{d-1,m}} \int_{-1}^{1} \cdots \int_{-1}^{1} \mathcal{P}_{\boldsymbol{i}}[f](\boldsymbol{x}) \mathrm{d}x_{i_1} \cdots \mathrm{d}x_{i_m}. \qquad (5.2)$$

Next, let $\tilde{f}(x_1, \ldots, x_{d-1}) = \int_{-1}^{1} x_d f(x_1, \ldots, x_d) \mathrm{d}x_d$. Since for every $\boldsymbol{i} \in U_{d-1,m-1}$

$$\begin{aligned}&\int_{-1}^{1} \cdots \int_{-1}^{1} \mathcal{P}_{\boldsymbol{i}}[\tilde{f}](\boldsymbol{x}) \mathrm{d}x_{i_1} \cdots \mathrm{d}x_{i_{m-1}} \\ &= \int_{-1}^{1} \cdots \int_{-1}^{1} x_{i_1} \cdots x_{i_{m-1}} x_d f_{x_{i_1} \cdots x_{i_{m-1}} x_d}(\boldsymbol{x}_{\tilde{\boldsymbol{i}}}) \mathrm{d}x_{i_1} \cdots \mathrm{d}x_{i_{m-1}} \mathrm{d}x_d \\ &= \int_{-1}^{1} \cdots \int_{-1}^{1} \mathcal{P}_{\tilde{\boldsymbol{i}}}[f](\boldsymbol{x}_{\tilde{\boldsymbol{i}}}) \mathrm{d}x_{i_1} \cdots \mathrm{d}x_{i_{m-1}} \mathrm{d}x_d,\end{aligned}$$

where $\tilde{\boldsymbol{i}} = [i_1, i_2, \ldots, i_{m-1}, d]$, and using again the induction assumption, we have

$$\begin{aligned}-I_{d-1}[\tilde{f}] &= \sum_{m=1}^{d} (-1)^m \sum_{\boldsymbol{i} \in U_{d-1,m-1}} \int_{-1}^{1} \cdots \int_{-1}^{1} \mathcal{P}_{\boldsymbol{i}}[\tilde{f}](\boldsymbol{x}) \mathrm{d}x_{i_1} \cdots \mathrm{d}x_{i_{m-1}} \\ &= \sum_{m=1}^{d} (-1)^m \sum_{\boldsymbol{i} \in U_{d-1,m-1}} \int_{-1}^{1} \cdots \int_{-1}^{1} \mathcal{P}_{\tilde{\boldsymbol{i}}}[f](\boldsymbol{x}) \mathrm{d}x_{i_1} \cdots \mathrm{d}x_{i_{m-1}} \mathrm{d}x_d. \qquad (5.3)\end{aligned}$$

Recalling the definition of $U_{d,m}$ as the set of all strictly monotone length-m sequences from $\{1, 2, \ldots, d\}$, it is clear that

$$U_{d-1,m} \cup \{\tilde{\boldsymbol{i}} \,:\, \boldsymbol{i} \in U_{d-1,m-1}\} = U_{d,m}$$

for $m = 1, \ldots, d-1$, with obvious corrections for $m = 0$ and $m = d$. Putting together (5.2) and (5.3), we thus deduce that

$$\hat{f}_{\mathbf{0}}^{[\mathbf{0}]} = I_d[f] = I_{d-1}[f_+] + I_{d-1}[f_-] - I_{d-1}[\tilde{f}]$$

indeed equals (5.1) and the proof is complete. □

The identity (5.1) replaces a single d-variate integral with 2^d integrals over different faces of the d-dimensional cube. This may seem as a poor bargain: Not so! Remember that we wish to recycle derivative values that we have already calculated in the context of extended Filon method: values of $f_{x_1x_2\cdots x_d}$ on a tartan grid and perhaps higher derivatives at the vertices. Clearly, this is not sufficient information for the computation of lower-grade coefficients and we are compelled to calculate f and its lower derivatives as well. Our intention, however, is to keep these calculations to an absolute minimum, while presenting general and usable theory, applicable to all grades. Paradoxically, the 2^d integrals in (5.1) provide a better organising principle for the task in hand than a single integral.

We wish to approximate m-fold integrals of the generic form

$$\mathcal{J}[h]=\int_{-1}^{1}\cdots\int_{-1}^{1}x_1\cdots x_m h_{x_1\cdots x_m}(x_1,\ldots,x_m)\mathrm{d}x_1\cdots\mathrm{d}x_m.$$

Assuming that g is analytic in $|z|\le 1$ and

$$h(x_1,\ldots,x_m)=\sum_{j_1=0}^{\infty}\cdots\sum_{j_m=0}^{\infty}\frac{h_{\boldsymbol{j}}}{\boldsymbol{j}!}\boldsymbol{x}^{\boldsymbol{j}},$$

where $h_{\boldsymbol{j}}=\partial_{\boldsymbol{x}}^{\boldsymbol{j}}h(\mathbf{0})$, we readily verify that

$$\begin{aligned}\mathcal{J}[h]&=\sum_{j_1=1}^{\infty}\cdots\sum_{j_m=1}^{\infty}\frac{h_{\boldsymbol{j}}}{(j_1-1)!\cdots(j_m-1)!}\int_{-1}^{1}\cdots\int_{-1}^{1}\boldsymbol{x}^{\boldsymbol{j}}\mathrm{d}x_1\cdots\mathrm{d}x_m\\&=2^m\sum_{j_1=0}^{\infty}\cdots\sum_{j_m=0}^{\infty}\frac{(2j_1)\cdots(2j_m)}{(2j_1+1)!\cdots(2j_m+1)!}h_{\boldsymbol{j}}\\&=2^m\left[\sum_{j_1=0}^{\infty}\frac{2j_1}{(2j_1+1)!}\partial_{x_1}^{2j_1}\right]\left[\sum_{j_2=0}^{\infty}\frac{2j_2}{(2j_2+1)!}\partial_{x_2}^{2j_2}\right]\cdots\left[\sum_{j_m=0}^{\infty}\frac{2j_m}{(2j_m+1)!}\partial_{x_m}^{2j_m}\right]h(\mathbf{0})\\&=2^m\prod_{j=1}^{m}\left(\frac{\partial_{x_j}\cosh\partial_{x_j}-\sinh\partial_{x_j}}{\partial_{x_j}^2}\right)h_{x_1x_2\cdots x_m}(\mathbf{0}).\end{aligned}$$

Let us assume that

$$\sum_{k=1}^{\nu}p_k\sinh r_k\theta=\frac{\theta\cosh\theta-\sinh\theta}{\theta^2}+\mathcal{O}\left(\theta^{\bar{p}+1}\right). \tag{5.4}$$

Then, recalling the proof of Theorem 6,

$$\sum_{k_1=1}^{\nu}\sum_{k_2=1}^{\nu}\cdots\sum_{k_m=1}^{\mu}\left(\prod_{j=1}^{m}p_{k_j}\right)\mathcal{S}_{\mathbf{0}}[h_{x_1x_2\cdots x_m}](r_{k_1},\ldots,r_{k_m})$$

coincides with $\mathcal{J}[h]$ for all polynomials h of degree $\bar{p}$ in each variable.

With greater generality, consider $\boldsymbol{i} \in U_{d,m}$. Examining (5.1) we observe that $\mathcal{S}_{\mathbf{1}}$ therein acts in any coordinate which is *not* in $i_1, i_2, \ldots, i_m$ while, by our analysis, $\mathcal{S}_{\mathbf{0}}$ above acts on the coordinates in $\boldsymbol{i}$. Altogether, we have an operator $\mathcal{S}$ that acts in all d coordinates and the quadrature

$$\mathcal{R}_{\boldsymbol{i}} = \sum_{k_1=1}^{\nu} \cdots \sum_{k_m=1}^{\nu} \left(\prod_{j=1}^{m} p_{k_j} \right) S_{\boldsymbol{\beta}(\boldsymbol{i})}[\partial_{\boldsymbol{x}}^{\mathbf{1}} f](\boldsymbol{r}_{\boldsymbol{i},\boldsymbol{k}}) \tag{5.5}$$

coincides with

$$\int_{-1}^{1} \cdots \int_{-1}^{1} \mathcal{P}_{\boldsymbol{i}}[f](\boldsymbol{x}) \mathrm{d}x_{i_1} \cdots \mathrm{d}x_{i_m}$$

for all polynomials f of order $\le \bar{p}$ in each variable. Here $\boldsymbol{r}_{\boldsymbol{i},\boldsymbol{k}}$ is obtained from $\boldsymbol{x}$ by replacing each x_{i_j} with r_{k_j} and filling-in the $d-m$ remaining coordinates with ones. Moreover, in $\boldsymbol{\beta}(\boldsymbol{i}) \in \mathbb{Z}_2^d$ we place 0 in the kth coordinate if there exists $i_j = k$, 1 otherwise. We adopt the convention that $\mathcal{R}_{[0]} = \mathcal{S}_{\mathbf{1}}[f](\mathbf{1})$. Combining (5.5) with (5.1), we thus approximate

$$\hat{f}_{\mathbf{0}}^{[\mathbf{0}]} \approx \sum_{m=0}^{d} (-1)^m \sum_{\boldsymbol{i} \in U_{d,m}} \mathcal{R}_{\boldsymbol{i}}. \tag{5.6}$$

Note that (5.6) uses derivatives $f_{x_{i_1} x_{i_2} \cdots x_{i_m}}$ on an m-dimensional tartan grid. For example, for $d = 3$, we need to compute f at the vertices (a 0-dimensional grid), f_{x_1}, f_{x_2} and f_{x_2} on lines (1-dimensional grids), $f_{x_1 x_2}, f_{x_1 x_3}$ and $f_{x_2 x_3}$ on squares (2-dimensional grids) and $f_{x_1 x_2 x_3}$ on the full 3-dimensional cube – except that the last (and most expensive) computation is anyway required for the implementation of extended Filon methods.

As an example, in $d = 2$ we approximate

$$\begin{aligned} \hat{f}_{0,0}^{[0,0]} \approx \mathcal{S}_{[1,1]}[f](1,1) &- \sum_{k_1=1}^{\nu} p_{k_1} \mathcal{S}_{[0,1]}[f_{x_1}](r_{k_1}, 1) - \sum_{k_2=1}^{\nu} p_{k_2} \mathcal{S}_{[1,0]}[f_{x_2}](1, r_{k_2}) \\ &+ \sum_{k_1=1}^{\nu} \sum_{k_2=1}^{\nu} p_{k_1} p_{k_2} \mathcal{S}_{[0,0]}[f_{x_1 x_2}](r_{k_1}, r_{k_2}). \end{aligned}$$

The approximation (5.5) can be generalised easily to cater for the situation when higher (odd) derivatives are available at the vertices. The idea is identical to the route that led from (4.11), say, to (4.16): In place of (5.4), we seek $p_1, \ldots, p_\nu$ and $\tilde{p}$ so that

$$\sum_{k=1}^{\nu} p_k \sinh r_k \theta + \tilde{p}\, \theta^2 \sinh \theta = \frac{\theta \cosh \theta - \sinh \theta}{\theta^2} + \mathcal{O}\big(\theta^{\bar{p}+1}\big)\,. \tag{5.7}$$

Exotic quadrature (5.6) is, as a matter of fact, more general and there is nothing to prevent us from applying it to *any* $\hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]}$, simply by replacing f with $f \prod_{j=1}^{d} u_{n_j}^{[\alpha_j]}(x_j)$. Of course, this makes little sense when $\max n_j$ is large, but provides an efficient approach for small $\max n_j$s.

In Table 4 we report the errors committed by (5.6), as applied no just to $\hat{f}_{\mathbf{0}}^{[\mathbf{0}]}$ but also to other values of $\boldsymbol{n}$. Clearly, for $\max n_j \le 1$ the results are excellent. However, already for the relatively ‘small’ $\boldsymbol{n} = [2, 3]$ the error exceeds by far that of even the simplest extended

$\boldsymbol{n}$	$\boldsymbol{\alpha}$	$\nu=3$	$\nu=4$
$[0,0]$	$[0,0]$	2.2608_{-07}	6.5700_{-12}
$[1,0]$	$[0,0]$	9.7521_{-05}	2.8998_{-09}
	$[1,0]$	2.7895_{-08}	1.3225_{-12}
$[1,1]$	$[0,0]$	3.5210_{-07}	8.3656_{-09}
	$[1,0]$	1.1722_{-04}	3.7876_{-08}
	$[0,1]$	6.2893_{-05}	1.8871_{-09}
	$[1,1]$	1.3636_{-06}	1.0923_{-10}
$[2,3]$	$[0,0]$	4.2482_{-03}	2.8663_{-03}

Table 4: Absolute value of the errors committed by the exotic quadrature (5.6) for four different $\boldsymbol{n}$s and $f(x,y)=\mathrm{e}^{x-2y}$.

Filon: the onset of asymptotic behaviour, underlying Filon-type methods, is very rapid indeed! Indeed, given that $\hat{f}_{2,3}^{[0,0]}\approx -9.0748_{-03}$, performance is hardly better than just setting this coefficient to zero.

Note that for $\nu=3$ we have used the values of r_1,r_2,r_3 that have been already mentioned in the previous section, and which result, consistently with (5.4), in

$$\boldsymbol{p}=\left[\begin{array}{ccc} \frac{11}{350}\frac{150-13\sqrt{15}}{\sqrt{495-66\sqrt{15}}} & \frac{11}{350}\frac{150+13\sqrt{15}}{\sqrt{495+66\sqrt{15}}} & \frac{1}{21}\end{array}\right].$$

The reason for this choice, as well as our choice of $\boldsymbol{r}$ and $\boldsymbol{p}$ for $\nu=4$, will become clear in Subsection 5.3.

Another pleasing feature apparent from Tables 3–4 is that extended Filon and exotic quadrature are in a sense complementary: when one is good, the other is bad and *vice versa*. This is fairly obvious from their distinct organising principles, since we have optimised extended Filon for oscillatory integrals and designed exotic quadrature to do well in non-oscillatory setting.

5.2 Higher-grade terms

To illustrate our methodology, consider the bivariate integral

$$\hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]}=\int_{-1}^{1}\int_{-1}^{1} f(x_1,x_2)u_{n_1}^{[\alpha_1]}(x_1)u_{n_2}^{[\alpha_2]}(x_2)\mathrm{d}x_1\mathrm{d}x_2,$$

where we assume that $n_2\geq 1$ is large enough (so that $u_{n_2}^{[\alpha_2]}$ oscillates rapidly) while $n_1\geq 0$ is small. The obvious idea is to combine our two techniques: extended Filon for the x_2 variable, exotic quadrature for x_1. Thus, letting $F(x_1,x_2)=f(x_1,x_2)u_{n_1}^{[\alpha_1]}(x_1)$, we have

$$\hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]}=\int_{-1}^{1}\left[\int_{-1}^{1}F(x_1,x_2)\mathrm{d}x_1\right]u_{n_2}^{[\alpha_2]}(x_2)\mathrm{d}x_2=\int_{-1}^{1}[F(1,x_2)+F(-1,x_2)]u_{n_2}^{[\alpha_2]}(x_2)\mathrm{d}x_2$$
$$-\int_{-1}^{1}\left[\int_{-1}^{1}x_1F_{x_1}(x_1,x_2)\mathrm{d}x_1\right]u_{n_2}^{[\alpha_2]}(x_2)\mathrm{d}x_2.$$

The obvious idea is to apply an extended Filon method in the single variable x_2 and exotic quadrature in the other variable. For example, we use $\mathcal{Q}^{[\alpha_2]}_{n,1,2,\nu}$ on the second component,

$$\int_{-1}^{1} h(x)u^{[\alpha_2]}_{n_2}(x)\mathrm{d}x \approx \frac{(-1)^{n_2+\alpha_2}}{(\pi\mu^{[\alpha_2]}_{n_2})^2}\mathcal{S}_{[\alpha_2]}[\partial_x h](1) - \frac{(-1)^{n_2+\alpha_2}}{(\pi\mu^{[\alpha_2]}_{n_2})^4}\sum_{k_2=1}^{\nu} a^{[\alpha_2,1]}_{k_2}\mathcal{S}_{[\alpha_2]}[\partial_x h](r_{k_2}),$$

while the two non-oscillatory terms are

$$F(1,x_2)+F(-1,x_2) = \mathcal{S}_{[1]}[F](1),$$
$$\int_{-1}^{1} x_1 F_{x_1}(x_1,x_2)\mathrm{d}x_1 \approx \sum_{k_1=1}^{\nu} p_{k_1}\mathcal{S}_{[1]}[\partial_{x_1}F](r_{k_1}).$$

To combine these two, we note that the operator $\mathcal{S}$ obeys a 'multiplication' rule which we have already used in the construction of quadrature formula (5.5): let $\boldsymbol{i}\in U_{d,m}$, $\boldsymbol{j}\in U_{d,d-m}$ so that the two vectors together comprise all of $\{1,2,\ldots,d\}$ (in other words, they are a partition of $\{1,2,\ldots,d\}$). Moreover, let $\boldsymbol{\gamma}\in\mathbb{Z}_2^m$, $\boldsymbol{\delta}\in\mathbb{Z}_+^{d-m}$, $\boldsymbol{\epsilon}\in\mathbb{Z}_+^m$ and $\boldsymbol{\kappa}\in\mathbb{Z}_+^{d-m}$. Then

$$\mathcal{S}_{\boldsymbol{\gamma}}[\partial^{\epsilon_1}_{x_{i_1}}\cdots\partial^{\epsilon_m}_{x_{i_m}}\mathcal{S}_{\boldsymbol{\delta}}[\partial^{\kappa_1}_{x_{j_1}}\cdots\partial^{\kappa_{d-m}}_{x_{j_{d-m}}} f](x_{j_1},\ldots,x_{j_{d-m}})](x_{i_1},\ldots,i_m) = \mathcal{S}_{\boldsymbol{\delta}}[\partial^{\boldsymbol{\omega}}_{\boldsymbol{x}} f](\boldsymbol{x}), \quad (5.8)$$

where $\boldsymbol{\delta}\in\mathbb{Z}_+^d$ is concatenation of the vectors $\boldsymbol{\gamma}$ and $\boldsymbol{\delta}$ in the natural order imposed by the concatenation of $\boldsymbol{i}$ and $\boldsymbol{j}$, while $\boldsymbol{\omega}\in\mathbb{Z}_+^d$ is the concatenation of $\boldsymbol{\epsilon}$ and $\boldsymbol{\kappa}$ in the same order: For example, letting $d=5$ and

$$\boldsymbol{i}=[1,3],\quad \boldsymbol{j}=[2,4,5],\qquad \boldsymbol{\gamma}=[0,1],\quad \boldsymbol{\delta}=[1,0,1],\qquad \boldsymbol{\epsilon}=[0,2],\quad \boldsymbol{\kappa}=[3,1,2],$$

we have

$$\mathcal{S}_{[0,1]}[\partial_{x_3}\mathcal{S}_{[1,0,1]}[\partial^3_{x_2}\partial_{x_4}\partial^2_{x_5} f](x_2,x_3,x_5)](x_1,x_3) = \mathcal{S}_{[0,1,1,0,1]}[\partial^3_{x_2}\partial^2_{x_3}\partial_{x_4}\partial^2_{x_5} f](\boldsymbol{x}).$$

Using (5.8), we combine exotic quadrature with extended Filon and the outcome is

$$\begin{aligned}\hat{f}^{[\boldsymbol{\alpha}]}_{\boldsymbol{n}} \approx{}& \frac{(-1)^{n_2+\alpha_2}}{(\pi\mu^{[\alpha_2]}_{n_2})^2}\left[\mathcal{S}_{[1,\alpha_2]}[\partial_{x_2}F](1,1) - \sum_{k_1=1}^{\nu} p_{k_1}\mathcal{S}_{[0,\alpha_2]}[\partial_{x_1}\partial_{x_2}F](r_{k_1},1)\right]\\ &- \frac{(-1)^{n_2+\alpha_2}}{(\pi\mu^{[\alpha_2]}_{n_2})^4}\left[\sum_{k_2=1}^{\nu} a^{[\alpha_2,1]}_{k_2}\mathcal{S}_{[1,\alpha_2]}[\partial_{x_2}F](1,r_{k_2})\right.\\ &\left. - \sum_{k_1=1}^{\nu}\sum_{k_2=1}^{\nu} p_{k_1}a^{[\alpha_2,1]}_{k_2}\mathcal{S}_{[0,\alpha_2]}[\partial_{x_1}\partial_{x_2}F](r_{k_1},r_{k_2})\right].\end{aligned} \quad (5.9)$$

If $F=f$ (i.e., in the case $n_1=0$) we are recycling the very same function and derivative values that we have already used in 'pure' extended Filon and exotic quadratures. If, however, $F=fu^{[\alpha_1]}_{n_1}$ for $n_1\geq 1$ then extra values are required: f on the tartan grid along the boundary and f_{x_2} on the bivariate tartan grid.

The generalisation to arbitrary $d\geq 1$ is easy in principle, although notation rapidly becomes complicated. Given $\boldsymbol{n}\in\mathbb{Z}_+^d$, we separate coordinates into 'slow' and 'fast': a good

$\boldsymbol{n}$	$\boldsymbol{\alpha}$	$\nu = 3$	$\nu = 4$
$[0, 5]$	$[0, 0]$	1.1595_{-05}	3.4146_{-05}
	$[0, 1]$	1.7025_{-04}	5.8883_{-05}
$[0, 10]$	$[0, 0]$	2.3932_{-06}	4.6557_{-07}
	$[0, 1]$	1.1273_{-05}	2.6272_{-07}

Table 5: Absolute value of the errors committed by a combination of extended Filon and exotic quadrature for two different values of $\boldsymbol{n}$ and $f(x, y) = \mathrm{e}^{x-2y}$.

strategy is to choose threshold $n^\star \geq 1$ and let each $n_k \leq n^\star - 1$ be 'slow', 'fast' otherwise. This partitions $\{1, 2, \ldots, d\}$ into $I_\mathrm{s} \cup I_\mathrm{f}$ and we set

$$F(\boldsymbol{x}) = f(\boldsymbol{x}) \prod_{i \in I_\mathrm{s}} u_{n_i}^{[\alpha_i]}(x_i).$$

Then

$$\hat{f}_{\boldsymbol{n}}^{[\boldsymbol{\alpha}]} = \int_{-1}^{1} \cdots \int_{-1}^{1} \left[\int_{-1}^{1} \cdots \int_{-1}^{1} F(\boldsymbol{x}) \prod_{i \in I_\mathrm{s}} \mathrm{d}x_i \right] \prod_{i \in I_\mathrm{f}} u_{n_i}^{[\alpha_i]}(x_i) \mathrm{d}x_i.$$

The idea is to discretise the integrals within square brackets with exotic quadrature and the integrals with respect to the 'fast' variables using extended Filon.

It is possible to describe this procedure explicitly and with full generality, but it rapidly leads to fairly complicated and opaque expressions. It is probably much more helpful to state it in words. Thus, we replace the inner non-oscillatory integral with a formula identical to (5.6), except that we act only on 'slow' variables: the 'fast' variables are retained intact. This results in an oscillatory integral in 'fast' variables, which we discretise with the extended Filon method $\mathcal{Q}_{\boldsymbol{n},N,M,\nu}^{[\boldsymbol{\alpha}]}$. Since both methods can be expressed in terms of the action of operators $\mathcal{S}$ on tartan grid extending over faces of $[-1, 1]^d$ of different dimensions, we use identity (5.8) to simplify the resulting method in a manner similar to (5.9).

In Table 5 we used a combination of extended Filon and exotic quadrature – actually, the scheme (5.9) – for two different values of $\boldsymbol{n}$ with $n_1 = 0$. (Thus, $F = f$.) Note that for $\boldsymbol{n} = [0, 5]$ taking $\nu = 4$ does not lead to much advantage (if at all) over $\nu = 3$: this is in all likelihood caused by the fact that the conditioning of vectors $\boldsymbol{a}^{[\alpha,1]}$ deteriorates rapidly with ν.

In our experience, if $\bar{n}$ is small, it is probably preferable to treat the entire integrand as F and employ d-variate exotic quadrature (similar to (5.6)), rather than mixing it with extended Filon. The reason is that, as we have already mentioned, the vectors $\boldsymbol{a}^{[\alpha,k]}$ might have large norms and this contributes significantly to error for low $\bar{n}$. Of course, mixed quadrature is unavoidable when $\bar{n} = 0$ (and we cannot use 'full' extended Filon), while $\max n_k \gg 1$ (hence the integrand oscillates rapidly).

5.3 Optimal coefficients $\boldsymbol{r}$

We use the freedom that we have in the choice of $r_1 < r_2 < \cdots < r_{\nu-1}$ to maximise the order $\bar{p}$ in (5.4).

Our first observation is that, similarly to the proof of Proposition 5, $\bar{p}$ is odd and (5.4) is equivalent to the linear conditions

$$\sum_{k=1}^{\nu} p_k r_k^{2m+1} = \frac{1}{2m+3}, \qquad m = 0, 1, \ldots, \frac{\bar{p}-3}{2}. \tag{5.10}$$

We identify the right-hand side of (5.10) with the mth moment of the Borel measure $\mathrm{d}\zeta(x) = \frac{1}{2}x^{\frac{1}{2}}\mathrm{d}x$, $x \in [0,1]$ – in other words,

$$\tfrac{1}{2}\int_0^1 x^{m+\frac{1}{2}}\mathrm{d}x = \frac{1}{2m+3}, \qquad m \in \mathbb{Z}_+.$$

Lemma 8 *Let $\zeta_{\nu,1} < \zeta_{\nu,2} < \cdots < \zeta_{\nu,\nu-1}$ be the zeros of the orthogonal polynomial of degree $\nu-1$ with respect to the measure $(1-x)\mathrm{d}\zeta(x)$, set $\zeta_\nu = 1$ and let $b_1, b_2, \ldots, b_\nu$ be the weights of the ν-point Radau quadrature with this measure. Then*

$$r_k = \sqrt{\zeta_{\nu,k}}, \quad p_k = \frac{b_k}{\sqrt{\zeta_{\nu,k}}}, \qquad k = 1, 2, \ldots, \nu.$$

Moreover, in that case $\bar{p} = 4\nu - 2$

Proof Recall that a Radau quadrature with the nodes $c_1 < c_2 < \ldots < c_\nu = 1$ is

$$\int_0^1 g(x)\mathrm{d}\zeta(x) \approx \sum_{k=1}^{\nu} b_k g(\zeta_{\nu,k}),$$

where $\zeta_{\nu,k}$s have been defined above and we can obtain the weights $b_1, \ldots, b_\nu$ by requiring that the formula is exact for $g(x) = x^{i-1}$, $i = 1, \ldots, \nu$: this results in a nonsingular Vandermonde system. Moreover, the method is of order $2\nu - 1$, i.e. exact for all polynomials g of order $\leq 2\nu - 2$ (Davis & Rabinowitz 1984). The lemma follows at once from (5.10). □

It is easy to identify the orthogonal polynomial in the statement of the lemma with the Jacobi polynomial $\mathrm{P}_{\nu-1}^{(1,\frac{1}{2})}$, shifted to the interval $[0,1]$. Note that, because of orthogonality, the coefficients $r_1, \ldots, r_{\nu-1}$ indeed reside in $(0,1)$, as required.

We have not managed to present optimal configuration of quadrature nodes for (5.7), a formula occurring when we incorporate higher derivatives, in terms of orthogonality conditions. Although it is possible to derive optimal r_ks for small ν by brute force, the general problem is open. It is just one of a long list of issues pertaining to the theory and computation with modified Fourier series in a cube that require much further attention.

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