Numerical quadrature of highly oscillatory integrals using derivatives

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Summary. Numerical approximation of highly oscillatory functions is an area of research that has received considerable attention in recent years. Using asymptotic expansions as a point of departure, we derive Filon-type and Levin-type methods. These methods have the wonderful property that they improve with accuracy as the frequency of oscillations increases. A generalization of Levin-type methods to integrals over higher dimensional domains will also be presented.

1 Introduction

A highly oscillatory integral is defined as

$$I[f] = \int_{\Omega} f e^{i\omega g} \, dV,$$

where f and g are smooth functions, $\omega \gg 1$ and Ω is some domain in $\mathbb{R}^d$. The parameter ω is a positive real number that represents the frequency of oscillations: large ω implies that the number of oscillations of $e^{i\omega g}$ in Ω is large. Furthermore, we will assume that g has no critical points; i.e., $\nabla g \neq 0$ in the closure of Ω. The goal of this paper is to numerically approximate such integrals, with attention paid to asymptotics, as $\omega \to \infty$.

For large values of ω, traditional quadrature techniques fail to approximate $I[f]$ efficiently. Each sample point for Gauss-Legendre quadrature is effectively a random value on the range of oscillation, unless the number of sample points is sufficiently greater than the number of oscillations. For the multivariate case, the number of sample points needed to effectively use repeated univariate quadrature grows exponentially with each dimension. In the univariate case with no stationary points, the integral $I[f]$ is $\mathcal{O}(\omega^{-1})$ for increasing ω [7]. This compares with an error of order $\mathcal{O}(1)$ when using Gauss-Legendre quadrature [1]. In other words, it is more accurate to approximate $I[f]$ by zero than to use Gauss-Legendre quadrature when ω is large! In this paper, we will demonstrate several methods for approximating $I[f]$ such that the accuracy improves as the frequency ω increases.

2 Univariate asymptotic expansion and Filon-type methods

This section consists of an overview of the relevant material from [1]. We focus on the case where $g' \neq 0$ in $[a,b]$, in other words there are no stationary points. The idea behind recent research into highly oscillatory integrals is to derive an asymptotic expansion for $I[f]$, which we then use to find the order of error of other, more efficient, methods. The key observation is that

$$\begin{aligned} I[f] &= \int_a^b f \mathrm{e}^{\mathrm{i}\omega g}\,\mathrm{d}x = \frac{1}{\mathrm{i}\omega}\int_a^b \frac{f}{g'}\frac{\mathrm{d}}{\mathrm{d}x}[\mathrm{e}^{\mathrm{i}\omega g}]\,\mathrm{d}x \\ &= \frac{1}{\mathrm{i}\omega}\left[\frac{f}{g'}\mathrm{e}^{\mathrm{i}\omega g}\right]_a^b - \frac{1}{\mathrm{i}\omega}\int_a^b \frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{f}{g'}\right]\mathrm{e}^{\mathrm{i}\omega g}\,\mathrm{d}x = Q[f] - \frac{1}{\mathrm{i}\omega} I\left[\left(\frac{f}{g'}\right)'\right], \end{aligned}$$

where $Q[f] = \frac{1}{\mathrm{i}\omega}\left[\frac{f}{g'}\mathrm{e}^{\mathrm{i}\omega g}\right]_a^b$. Note that the integral in the error term is $\mathcal{O}(\omega^{-1})$ [7], hence $Q[f]$ approximates $I[f]$ with an error of order $\mathcal{O}(\omega^{-2})$. Moreover, the error term is another highly oscillatory integral, hence we can use $Q[f]$ to approximate it as well. Clearly, by continuing this process, we derive the following asymptotic expansion:

$$I[f] \sim \sum_{k=1}^{\infty} \frac{1}{(\mathrm{i}\omega)^k}\left(\sigma_k[f](b)\mathrm{e}^{\mathrm{i}\omega g(b)} - \sigma_k[f](a)\mathrm{e}^{\mathrm{i}\omega g(a)}\right),$$

where

$$\sigma_1[f] = \frac{f}{g'}, \qquad \sigma_{k+1}[f] = \frac{\sigma_k[f]'}{g'}, \qquad k \geq 1.$$

Note that, if f and its first $s-1$ derivatives are zero at the endpoints, then the first s terms of this expansion are zero and $I[f] \sim \mathcal{O}(\omega^{-s-1})$.

We could, of course, use the partial sums of the asymptotic expansion to approximate $I[f]$. This approximation would improve with accuracy, the larger the frequency of oscillations ω. Unfortunately, the expansion will not typically converge for fixed ω, and there is a limit to how accurate the approximation can be. Hence we derive a Filon-type method. The idea is to approximate f by v using Hermite interpolation, i.e., v is a polynomial such that

$$v(x_k) = f(x_k), v'(x_k) = f'(x_k), \ldots, v^{(m_k-1)}(x_k) = f^{(m_k-1)}(x_k),$$

for some set of nodes $\{x_0, \ldots, x_\nu\}$ and multiplicities $\{m_0, \ldots, m_\nu\}$, and $k = 0, 1, \ldots, x_\nu$. If the moments of $\mathrm{e}^{\mathrm{i}\omega g}$ are available, then we can calculate $I[v]$ explicitly. Thus define $Q^F[f] = I[v]$. This method has an error

$$I[f] - Q^F[f] = I[f] - I[v] = I[f-v] = \mathcal{O}(\omega^{-s-1}),$$

where $s = \min\{m_0, m_\nu\}$. This follows since f and the first $s-1$ derivatives are zero at the endpoints, thus the first s terms of the asymptotic expansion are zero. Because the accuracy of $Q^F[f]$ depends on the accuracy of v interpolating f, adding additional sample points and multiplicities will typically decrease the error.

3 Univariate Levin-type method

Another method for approximating highly oscillatory integrals was developed by Levin in [3]. This method uses collocation instead of interpolation, removing the requirement that moments are computable. If there exists a function F such that $\frac{\mathrm{d}}{\mathrm{d}x}[F\mathrm{e}^{\mathrm{i}\omega g}] = f\mathrm{e}^{\mathrm{i}\omega g}$, then

$$I[f] = \int_a^b f\mathrm{e}^{\mathrm{i}\omega g}\,\mathrm{d}x = \int_a^b \frac{\mathrm{d}}{\mathrm{d}x}[F\mathrm{e}^{\mathrm{i}\omega g}]\mathrm{d}x = \left[F\mathrm{e}^{\mathrm{i}\omega g}\right]_a^b.$$

We can rewrite the condition as $\mathcal{L}[F] = f$ for the operator $\mathcal{L}[F] = F' + \mathrm{i}\omega g' F$. Hence we approximate F by some function v using collocation, i.e., if $v = \sum c_k \psi_k$ is a linear combination of basis functions $\{\psi_k\}$, then we solve for $\{c_k\}$ using the system $\mathcal{L}[v](x_j) = f(x_j)$, at some set of points $\{x_0, \ldots, x_\nu\}$. We can then define the approximation to be

$$Q^L[f] = \int_a^b \mathcal{L}[v]\mathrm{e}^{\mathrm{i}\omega g}\,\mathrm{d}x = \int_a^b \frac{\mathrm{d}}{\mathrm{d}x}[v\mathrm{e}^{\mathrm{i}\omega g}]\mathrm{d}x = \left[v\mathrm{e}^{\mathrm{i}\omega g}\right]_a^b.$$

In [4], the current author generalized this method to include multiplicities, i.e., to each sample point x_j associate a multiplicity m_j. This results in the system

$$\mathcal{L}[v](x_j) = f(x_j), \mathcal{L}[v]'(x_j) = f'(x_j), \ldots, \mathcal{L}[v]^{(m_j-1)}(x_j) = f^{(m_j-1)}(x_j), \quad (1)$$

for $j = 0, 1, \ldots, \nu$. If every multiplicity m_j is one, then this is equivalent to the original Levin method. As in a Filon-type method, if the multiplicities at the endpoint are greater than or equal to s, then $I[f] - Q^L[f] = \mathcal{O}\big(\omega^{-s-1}\big)$, subject to the regularity condition. This condition states that the basis $\{g'\psi_k\}$ can interpolate at the given nodes and multiplicities.

To prove that $Q^L[f]$ has an asymptotic order of $\mathcal{O}\big(\omega^{-s-1}\big)$, we look at the error term $I[f] - Q^L[f] = I[f - \mathcal{L}[v]]$. If we can show that $\mathcal{L}[v]$ and its derivatives are bounded for increasing ω, the order of error will follow from the asymptotic expansion. Let A be the matrix associated with the system (1), in other words $A\mathbf{c} = \mathbf{f}$, where $\mathbf{c} = [c_0, \cdots, c_n]^\top$, and $\mathbf{f}$ is the vector associated with the right-hand side of (1). We can write $A = P + \mathrm{i}\omega G$, where P and G are independent of ω, and G is the matrix associated with interpolating at the given nodes and multiplicities by the basis $\{g'\psi_k\}$. Thence $\det A = (\mathrm{i}\omega)^{n+1} \det G + \mathcal{O}(\omega^n)$. The regularity condition ensures that $\det G \neq 0$, thus $\det A \neq 0$ and $(\det A)^{-1} = \mathcal{O}\big(\omega^{-n-1}\big)$. Cramer's rule states that $c_k = \frac{\det D_k}{\det A}$, where D_k is the matrix A with the $(k+1)$th column replaced by $\mathbf{f}$. Since

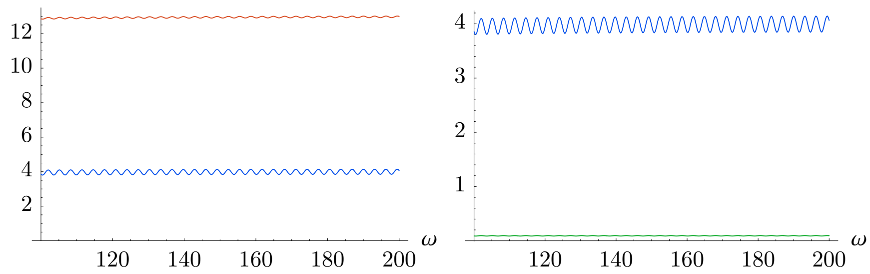

Fig. 1. The error scaled by ω^3 of the asymptotic expansion (left figure, top), $Q^L[f]$ (left figure, bottom)/(right figure, top) and $Q^F[f]$ (right figure, bottom) both with only endpoints and multiplicities two, for $I[f] = \int_0^1 \cosh x \, \mathrm{e}^{\mathrm{i}\omega\left(x^2+x\right)} \mathrm{d}x$.

D_k has one row independent of ω, $\det D_k = \mathcal{O}(\omega^{-n})$, and it follows that $c_k = \mathcal{O}\left(\omega^{-1}\right)$. Thus $\mathcal{L}[v] = \mathcal{O}(1)$, for $\omega \to \infty$.

Unlike a Filon-type method, we do not need to compute moments in order to compute $Q^L[f]$. Furthermore, if g has no stationary points and the basis $\{\psi_k\}$ is a Chebyshev set [6]—such as the standard polynomial basis $\psi_k(x) = x^k$—then the regularity condition is always satisfied. This follows since, if $\{\psi_k\}$ is a Chebyshev set, then $\{g'\psi_k\}$ is also a Chebyshev set.

The following example will demonstrate the effectiveness of this method. Consider the integral $\int_0^1 \cosh x \, \mathrm{e}^{\mathrm{i}\omega\left(x^2+x\right)} \mathrm{d}x$, in other words, $f(x) = \cosh x$ and $g(x) = x^2 + x$. We have no stationary points and moments are computable, hence all the methods discussed so far are applicable. We compare the asymptotic method with a Filon-type method and a Levin-type method, each with nodes $\{0, 1\}$ and multiplicities both two. For this choice of f and g, the Levin-type method is a significant improvement over the asymptotic expansion, whilst the Filon-type method is even more accurate. Not pictured is what happens when additional nodes and multiplicities are added. Adding additional nodes at $\frac{1}{4}$, $\frac{1}{2}$ and $\frac{3}{4}$ with multiplicities all one causes the error of the Levin-type method to drop to roughly equivalent to the current Filon-type method, whilst the error of the Filon-type method decreases even more, to approximately $10^{-5}\omega^{-3}$.

As an example of an integral for which a Filon-type method will not work, consider the case where $f(x) = \log(x+1)$ with oscillator $g(x) = \mathrm{e}^x \sin x$. This oscillator is sufficiently complicated so that the moments are unknown. On the other hand, a Levin-type method works wonderfully, as seen in Figure 2. This figure compares the errors of the asymptotic expansion with a levin-type method collocating at only the endpoints and a levin-type method collocating at the endpoints and the midpoint, where all multiplicities are one.

Unlike a Filon-type method, there is no reason we need to use polynomials for our collocation basis. By choosing our basis wisely we can significantly decrease the error, and, surprisingly, increase the asymptotic order. We define

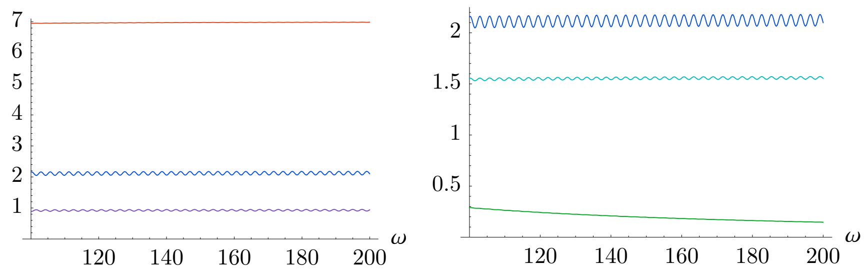

Fig. 2. The error scaled by ω^3 of the asymptotic expansion (left figure, top), $Q^L[f]$ collocating at the endpoints with multiplicities two (left figure, middle)/(right figure, top), $Q^L[f]$ collocating at the endpoints with multiplicities two and midpoint with multiplicity one (left figure, bottom), $Q^L[f]$ with asymptotic basis collocating at endpoints with multiplicities one (right figure, middle) and $Q^L[f]$ with asymptotic basis collocating at endpoints and midpoint with multiplicity one (right figure, bottom), for $I[f] = \int_0^1 \log(x+1) \mathrm{e}^{\mathrm{i}\omega \mathrm{e}^x \sin x} \mathrm{d}x$.

the asymptotic basis, named after its similarity to the terms in the asymptotic expansion, as:

$$\psi_0 = 1, \qquad \psi_1 = \frac{f}{g'}, \qquad \psi_{k+1} = \frac{\psi_k'}{g'}, \qquad k = 1, 2, \ldots .$$

It turns out that this choice of basis results in an order of error of $\mathcal{O}\left(\omega^{-n-s-1}\right)$, where $n+1$ is equal to the number of equations in the collocation system (1), assuming that the regularity condition is satisfied. This has the wonderful property that adding collocation points within the interval of integration increases the order. See [4] for a proof of the order of error. The right-hand side of Figure 2 demonstrates the effectiveness of this choice of basis. Many more examples can be found in [4].

4 Multivariate Levin-type method

In this section, based on work from [5], we will discuss how to generalize Levin-type methods for integrating

$$I_g[f, \Omega] = \int_\Omega f \mathrm{e}^{\mathrm{i}\omega g} \, \mathrm{d}V,$$

where $\Omega \subset \mathbb{R}^d$ is a multivariate piecewise smooth domain and g has no critical points in the closure of Ω, i.e., $\nabla g \neq 0$. We emphasize the dependence of I on g and Ω in this section, as we will need to deal with multiple oscillators in order to derive a Levin-type method. We will similarly denote a univariate Levin-type method as $Q_g^L[f, \Omega]$, for $\Omega = (a, b)$. For simplicity we will demonstrate

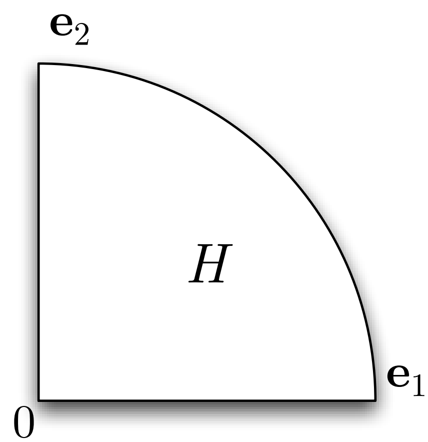

Fig. 3. Diagram of a unit quarter circle H.

how to derive a multivariate Levin-type method on a two-dimensional quarter unit circle H as seen in Figure 3, though the technique discussed can readily be generalized to other domains—including higher dimensional domains.

The asymptotic expansion and Filon-type methods were generalized to higher dimensional simplices and polytopes in [2]. Suppose that Ω is a polytope such that the oscillator g is not orthogonal to the boundary of Ω at any point on the boundary, which we call the non-resonance condition. From [2] we know that there exists an asymptotic expansion of the form

$$I_g[f,\Omega] \sim \sum_{k=0}^{\infty} \frac{1}{(-\mathrm{i}\omega)^{k+d}} \Theta_k[f], \tag{2}$$

where $\Theta_k[f]$ depends on f and its partial derivatives of order less than or equal to k, evaluated at the vertices of Ω. Hence, if we interpolate f by a polynomial v at the vertices of Ω with multiplicities at least $s-1$, then $I[f-v] = \mathcal{O}\big(\omega^{-s-d}\big)$.

We will now use this asymptotic expansion to construct a multivariate Levin-type method. In the univariate case, we determined the collocation operator $\mathcal{L}$ using the fundamental theorem of calculus. We mimic this by using the Stokes' theorem. Define the differential form $\rho = v(x,y)\mathrm{e}^{\mathrm{i}\omega g(x,y)}(\mathrm{d}x + \mathrm{d}y)$, where $v(x,y) = \sum c_k \psi_k(x,y)$ for some basis $\{\psi_k\}$. Then

$$\begin{aligned} \mathrm{d}\rho &= (v_x + \mathrm{i}\omega g_x v)\mathrm{e}^{\mathrm{i}\omega g}\mathrm{d}x \wedge \mathrm{d}y + (v_y + \mathrm{i}\omega g_y v)\mathrm{e}^{\mathrm{i}\omega g}\mathrm{d}y \wedge \mathrm{d}x \\ &= (v_x + \mathrm{i}\omega g_x v - v_y - \mathrm{i}\omega g_y v)\mathrm{e}^{\mathrm{i}\omega g}\mathrm{d}x \wedge \mathrm{d}y. \end{aligned}$$

Define the collocation operator $\mathcal{L}[v] = v_x + \mathrm{i}\omega g_x v - v_y - \mathrm{i}\omega g_y v$. For some sequence of nodes $\{\mathbf{x}_0, \ldots, \mathbf{x}_\nu\} \subset \mathbb{R}^2$ and multiplicities $\{m_0, \ldots, m_\nu\}$, we can determine the coefficients c_k by solving the system

$$\mathcal{D}^{\mathbf{m}}\mathcal{L}[v](\mathbf{x}_k) = \mathcal{D}^{\mathbf{m}} f(\mathbf{x}_k), \qquad 0 \le |\mathbf{m}| \le m_k - 1, \qquad k = 0, 1, \ldots, \nu, \tag{3}$$

where $\mathbf{m} \in \mathbb{N}^2$, $|\mathbf{m}|$ is the sum of the rows of the vector $\mathbf{m}$ and $\mathcal{D}^{\mathbf{m}}$ is the partial derivative operator. We then obtain, using $T_1(t) = [\cos t, \sin t]^\top$, $T_2(t) = [0, 1-t]^\top$, and $T_3(t) = [t, 0]^\top$ as the positively oriented boundary,

$$\begin{aligned}
I_g[f, \Omega] \approx I_g[\mathcal{L}[v], \Omega] &= \iint_H \mathrm{d}\rho = \oint_{\partial H} \rho = \oint_{\partial H} v \mathrm{e}^{\mathrm{i}\omega g}(\mathrm{d}x + \mathrm{d}y) \\
&= \int_0^{\frac{\pi}{2}} v(T_1(t))\mathrm{e}^{\mathrm{i}\omega g(T_1(t))}\,[1,1]\,T_1'(t)\,\mathrm{d}t \\
&\qquad + \int_0^1 v(T_2(t))\mathrm{e}^{\mathrm{i}\omega g(T_2(t))}\,[1,1]\,T_2'(t)\,\mathrm{d}t \\
&\qquad + \int_0^1 v(T_3(t))\mathrm{e}^{\mathrm{i}\omega g(T_3(t))}\,[1,1]\,T_3'(t)\,\mathrm{d}t \\
&= \int_0^{\frac{\pi}{2}} v(\cos t, \sin t)\mathrm{e}^{\mathrm{i}\omega g(\cos t, \sin t)}(\cos t - \sin t)\,\mathrm{d}t \qquad (4) \\
&\qquad - \int_0^1 v(0, 1-t)\mathrm{e}^{\mathrm{i}\omega g(0,1-t)}\,\mathrm{d}t + \int_0^1 v(t,0)\mathrm{e}^{\mathrm{i}\omega g(t,0)}\,\mathrm{d}t.
\end{aligned}$$

This is the sum of three univariate highly oscillatory integrals, with oscillators $\mathrm{e}^{\mathrm{i}\omega g(\cos t, \sin t)}$, $\mathrm{e}^{\mathrm{i}\omega g(0,1-t)}$, and $\mathrm{e}^{\mathrm{i}\omega g(t,0)}$. If we assume that these three oscillators have no stationary points, then we can approximate each of these integrals with a univariate Levin-type method, as described above. Hence we define:

$$Q_g^L[f, H] = Q_{g_1}^L[f_1, \left(0, \frac{\pi}{2}\right)] + Q_{g_2}^L[f_2, (0,1)] + Q_{g_3}^L[f_3, (0,1)],$$

for

$$\begin{aligned}
f_1(t) &= v(\cos t, \sin t)(\cos t - \sin t), & g_1(t) &= g(\cos t, \sin t), \\
f_2(t) &= -v(0, 1-t), & g_2(t) &= g(0, 1-t), \\
f_3(t) &= v(t, 0), & g_3(t) &= g(t, 0).
\end{aligned}$$

For the purposes of proving the order, we assume that the multiplicity at each endpoint of these univariate Levin-type methods is equal to the multiplicity at the point mapped to by the respective T_k.

Note that requiring that the univariate oscillators be free of stationary points is equivalent to requiring that ∇g is not orthogonal to the boundary of H, i.e., the non-resonance condition. Indeed,

$$\nabla g(T_k(t))^\top T_k'(t) = (g \circ T_k)'(t) = g_k'(t),$$

hence $g_k'(\xi) = 0$ if and only if ∇g is orthogonal to the boundary of H at the point $T_k(\xi)$. We also have a multivariate version of the regularity condition, which simply states that each univariate Levin-type method satisfies the regularity condition, and that the two-dimensional basis $\{(g_x - g_y)\psi_k\}$ can interpolate f at the given nodes and multiplicities. It turns out, subject to the non-resonance condition and the regularity condition, that $I_g[f, H] - Q_g^L[f, H] =$

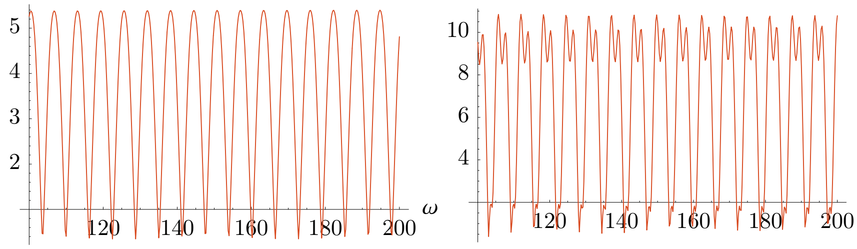

Fig. 4. The error scaled by ω^3 of $Q_g^L[f,H]$ collocating only at the vertices with multiplicities all one (left), and the error scaled by ω^4 collocating at the vertices with multiplicities two and the point $\left[\frac{1}{3},\frac{1}{3}\right]$ with multiplicity one (right), for $I_g[f,H] = \int_H \cos(x-2y)\, \mathrm{e}^{\mathrm{i}\omega(x^2+x-y)}\, \mathrm{d}V$.

$\mathcal{O}\big(\omega^{-s-2}\big)$, for s equal to the minimum of the multiplicities at the vertices of H.

From [5], we know that the asymptotic expansion (2) can be generalized to the non-polytope domain H, depending on the vertices of H. Hence we first show that $I_g[f,H] - I_g[\mathcal{L}[v],H] = \mathcal{O}\big(\omega^{-s-2}\big)$. The proof of this is almost identical to univariate case. We show that $\mathcal{L}[v]$ is bounded for increasing ω. As before the system (3) can be written as $A\mathbf{c} = \mathbf{f}$, where again $A = P + \mathrm{i}\omega G$ for matrices P and G independent of ω, and G is the matrix associated with interpolation at the given nodes and multiplicities by the basis $\{(g_x - g_y)\psi_k\}$. The new regularity condition ensures that $\det G \neq 0$, hence, again due to Cramer's rule, each c_k is of order $\mathcal{O}\big(\omega^{-1}\big)$. Thus $\mathcal{L}[v] = \mathcal{O}(1)$ for increasing ω, and the asymptotic expansion shows that $I_g[f,H] - I_g[\mathcal{L}[v],H] = I_g[f - \mathcal{L}[v],H] = \mathcal{O}\big(\omega^{-s-2}\big)$.

We now show that $I_g[\mathcal{L}[v],H] - Q_g^L[f,H] = \mathcal{O}\big(\omega^{-s-2}\big)$. Note that (4) is equal to $I_g[\mathcal{L}[v],H]$. But we know that each integrand f_k is of order $\mathcal{O}\big(\omega^{-1}\big)$. It follows that when we approximate these integrals using Q^L the error is of order $\mathcal{O}\big(\omega^{-s-2}\big)$. A proof for general domains, as well as a generalization of the asymptotic basis, can be found in [5].

We now demonstrate the effectiveness of this method. Consider the case where $f(x,y) = \cos(x-2y)$, with oscillator $g(x,y) = x^2 + x - y$. The univariate integrals will have oscillators $g_1(t) = \cos^2 t + \cos t - \sin t$, $g_2(t) = t - 1$, and $g_3(t) = t^2 + t$. Since these oscillators are free from stationary points, the non-resonance condition is satisfied. If we collocate at the vertices with multiplicities all one, then we obtain the left-hand side of Figure 4. Increasing the multiplicities to two and adding the interpolation point $\left[\frac{1}{3},\frac{1}{3}\right]$ with multiplicity one gives us the right-hand side. This results in the order increasing by one. More examples can be found in [5].

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