Andreas Asheim

Numerical Methods for Highly Oscillatory Problems

Doctoral thesis for the degree of philosophiae doctor

Trondheim, May 2010

Norwegian University of Science and Technology Faculty of Information Technology, Mathematics and Electrical Engineering Department of Mathematical Sciences



NTNU

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Preface

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> Andreas Asheim Trondheim, May 2010

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Chapter 1

Introduction

"Divergente Rekker ere i det Hele noget Fandensskab,og det er en Skam at man vover at grunde nogen Demonstration derpaa." -N. H. Abel in letter to Holmboe, 1928.

Classical numerical analysis has mainly revolved around a simple notion of continuity, typically that functions are "simple" when viewed on a small scale. More specifically there would be an underlying assumption on regularity in the asymptotic regime $h \to 0$, where h is a scale in e.g. time or space. In many ways this is a natural way to think since most physical models, especially those considered in engineering applications, are indeed regular in this limit. The boundary between asymptotic analysis and numerical analysis constitutes one of the less explored fields of applied mathematics, not counting honorable exceptions like the analysis of stiff ODE-problems. The idea that some phenomena should be considered in other limits than $h \rightarrow 0$ is old, and the associated techniques have proven of great use to physicists since the time of Newton. Notions of tolerances, error control and efficiency, central to the numerical analyst, have however seemed quite incompatible with these classical asymptotic techniques. A challenge, it has been pointed out, has therefore been to construct numerical methods that incorporate asymptotic characteristics, while at the same time improving accuracy over the classical techniques, and providing e.g. error control. The recent surge in attention on oscillatory problems and numerical techniques for these has resulted in remarkable methods that in certain cases show dramatic improvement in efficiency over both classical asymptotic and numerical techniques. The success of these techniques is rooted in the fact that they employ, often implicitly, techniques for resolving two different asymptotic regimes, e.g. high oscillations and a slowly varying envelope.

The problem with classical numerical quadrature methods applied to highly

oscillatory functions is quite obvious. Such methods typically work by approximating the integrand on an element of a partition, resolving the integral of the approximate integrand and finally summing over the partition. Clearly, if the frequency of the oscillation increases, the size of the partition must decrease in order to accurately resolve the integrand, thus increasing the computational load. Indeed, codes that have been touted as oscillatory quadrature methods have typically employed some way of tracking oscillations and applying a standard method on each period of oscillation. In other words, the idea that less resolution power is actually needed the more oscillations there are has not been prominent in numerics.

Classical asymptotic techniques for oscillatory integrals include examples like the method of stationary phase, the method of steepest descent and related saddle point methods[30]. Such methods yield asymptotic expansions of the considered integral. These expansions are typically non-convergent and can only give a limited accuracy. Not until recently, with the advent of more sophisticated numerical methods like e.g. Levin-type methods[20, 27], Filon-type methods[16, 17] and numerical steepest descent[11], has this been seen as a surmountable problem. These numerical techniques have the property that a number of terms in the asymptotic expansion of the error are zero, while at the same time large scale structure is resolved. If applied correctly, such methods exhibit convergence both in the regime $h \rightarrow 0$ and $\omega \rightarrow \infty$. Also, less computational effort is needed for such methods the more oscillations there are.

The issue of numerical versus asymptotic approximations of integrals has a direct analogue in the field of wave scattering. A wave scattering problem is typically modeled with a wave equation or Helmholtz equation, and a discretisation with e.g. finite elements or spectral methods corresponds to a classical $h \rightarrow 0$ approach. The Helmholtz equation can as well in some cases be reformulated as an integral equation, which in turn can be discretised using boundary elements. However good these methods are they will run into the problem of sampling requirements when the frequency of oscillation increases. Therefore, just as in the case of classical quadrature methods, the computational effort grows with increasing frequency. Again asymptotic techniques provide approximations that are more accurate with increasing frequency. The most basic of these being the well known Geometric Optics approximation(GO). More sophisticated techniques like Physical Optics and Geometrical Theory of Diffraction(GTD)[18] are used extensively in physics and engineering. All these methods are however not applicable, i.e. they are limited in accuracy, at moderately low wavenumbers and across Stokes lines.

In this work different aspects of the application of highly oscillatory quadrature have been considered. A central topic is the scattering by a smooth obstacle for which highly oscillatory quadrature methods open up a new viewpoint. In this introductory chapter a short review of a collection of themes relevant to this thesis, relating to highly oscillatory problems is presented. A summary of the papers and the papers themselves follow suit.

1.1 Oscillatory integrals and asymptotics

The model problem in oscillatory integration is the integral

$$\mathcal{I}[f] = \int_{a}^{b} f(x)e^{i\omega g(x)} \mathrm{d}x.$$
(1.1)

 ω is here a parameter that can be large. In that case the appropriate asymptotic regime being $\omega \to \infty$. f and g are functions assumed to be non-oscillatory, often called the envelope and the oscillator of the integral. A number of assumptions may be imposed on f and g, typically that they are n time differentiable in the interior of [a, b], or that there exist analytic continuations of them in certain parts of the complex plane.

The asymptotics of integrals of the form (1.1) is thoroughly treated in the literature, see e.g. [24, 30], a key characteristic being the localisation of the integral. By localisation we mean that asymptotically the value of the integral depends only on f and g and their derivatives at a discrete set of points. These are the endpoints of the interval, points of discontinuity of any derivative of f or g and the stationary points. Stationary points, often referred to as critical points, are points $\xi \in [a, b]$ such that $g'(\xi) = 0$. The number of derivatives that vanish at a stationary point we call the order of the stationary point. Thus, for example, we have the canonical function $g(x) = x^n$, which possesses an order n - 1 stationary point at the origin.

Case of no stationary points

In the case where $f, g \in C^{\infty}[a, b]$ and $g'(x) \neq 0$, $x \in [a, b]$, the full asymptotic expansion of (1.1) is easily obtained by iterated integration by parts, which gives a full asymptotic expansion,

$$\mathcal{I}[f] \sim -\sum_{m=1}^{\infty} \frac{1}{(-i\omega)^m} \left[\frac{e^{i\omega g(b)}}{g'(b)} \sigma_{m-1}[f](b) - \frac{e^{i\omega g(a)}}{g'(a)} \sigma_{m-1}[f](a) \right], \quad (1.2)$$

where

$$\sigma_0[f](x) = f(x) \sigma_{m+1}[f](x) = \frac{d}{dx} \frac{\sigma_m[f](x)}{g'(x)}, \quad m = 0, 1, \dots$$
(1.3)

From this expansion we immediately see the above mentioned localisation; the asymptotics depend only on f and g at the endpoints of the interval [a, b].

Case of stationary points

If we have at least one point $\xi \in [a, b]$ such that $g'(\xi) = 0$ the situation is quite different. In this case, the integration by parts procedure will fail since the function f/g' is not continuously differentiable. Several other approaches may yield the asymptotic expansion of the integral in such cases. For example will the stationary phase approximation[30] give the leading order term with no great effort. Higher order terms can also be found, but not as easily.

As suggested by Iserles & Nørsett[16], one useful way of expanding the integral in the case where there are stationary points is a simple add- and subtract procedure. For example, when there is a single stationary point $\xi \in [a, b]$ of order one, then,

$$\mathcal{I}[f] = f(\xi)\mathcal{I}[1] + \mathcal{I}[f - f(\xi)],$$

and the second integral can be treated with integration by parts since $(f - f(\xi))/g'$ has a removable singularity. More generally, the singularity induced by a stationary point of order s is removable when subtracting an s-term Taylor expansion of f:

$$\mathcal{I}[f] = \sum_{j=0}^{s-1} \frac{1}{j!} f^{(j)}(\xi) \mathcal{I}[(\cdot - \xi)^j] + \int_a^b \left(f(x) - \sum_{j=0}^{s-1} \frac{1}{j!} f^{(j)}(\xi) (x - \xi)^j \right) e^{i\omega g(x)} \mathrm{d}x.$$

This leads to an expansion, sometimes referred to as the Iserles-Nørsett expansion, of the integral of the form (1.2) plus a sum of so-called generalised moments, $\mathcal{I}[(\cdot - \xi)^j], j = 0, \ldots, s - 1$. Though expressed in terms of oscillatory integrals this expansion is useful for analysing numerical methods.

The method of steepest descent

For finding a more pure-bred asymptotic expansion the method of steepest descent is a very powerful tool. The method of steepest descent provides an algorithm for obtaining the asymptotics for a wide range of oscillatory integrals, including cases of stationary points. Assuming the functions f and g have complex analytic(holomorphic) extensions in the complex plane, the method of steepest descent involves deforming the path of integration into the complex plane. As a consequence of Cauchy's Integral Theorem[9] and the analytic properties of f and g, we have

$$\int_{a}^{b} f(x)e^{i\omega g(x)} \mathrm{d}x = \int_{\Gamma} f(x)e^{i\omega g(x)} \mathrm{d}s_{x},$$

where $\Gamma \in \mathbb{C}$ is a curve that starts at a and ends at b. Of particular interest are paths along which the integrand is non-oscillatory. A path of steepest descent¹ is a curve in the complex plane, described by the function $h_x(p)$, which is defined by the equation

$$g(h_x(p)) = g(x) + ip, \qquad p \le 0,$$
 (1.4)

along with the condition that $h_x(0) = x$. $h_x(p)$ then starts at $x \in \mathbb{R}$ and runs into the complex plane in such a way that $e^{i\omega g(h_x(p))} = e^{i\omega g(x)}e^{-\omega p}$, rendering the integrand non-oscillatory and exponentially decreasing. Equation (1.4) is uniquely solvable, at least in a neighborhood of x, provided that $g'(x) \neq 0$. In case x is an order s stationary point there are s + 1 steepest-descent directions from x^2 .

When x is a stationary point we must have a rule to select which solution branch of (1.4) to take. Assume now that g is strictly monotone in the interval (a, b), possibly with stationary points at a or b. The following argument can be extended to more general configurations by subdividing the interval such that all stationary points are endpoints. The path of steepest descent originating at a will never meet the path of steepest descent starting at b; along a path of steepest descent starting at x we have that real $(g) \equiv g(x)$, and $g(a) \neq g(b)$ by the monotonicity of g. Now it proves useful to consider the *ridges* and *valleys* of the analytical extension of g. Briefly, two points are in the same valley if they can be connected by a path which does not intersect the real line and along which imag(g) is positive(negative for ridges). This corresponds nicely to our earthly notions of valleys and ridges. If now two paths of steepest descent follow the same valley, it can be shown that the integral along the path connecting the point $h_a(P)$ and $h_b(P)$ is exponentially small in ω , and it vanishes as $P \to \infty$. This provides a criterion for choosing the right path among the s + 1 available at a stationary point.

The procedure yields the following decomposition of the integral,

$$\mathcal{I}[f] = \mathcal{I}[f; h_a] - \mathcal{I}[f; h_b], \qquad (1.5)$$

where,

$$\mathcal{I}[f;h_x] = e^{i\omega g(x)} \int_0^\infty f(h_x(p)) h'_x(p) e^{-\omega p} \mathrm{d}p.$$
(1.6)

Note that the integrals, one for each contributing point, are of Laplace type, and an asymptotic expansion can therefore be found by standard methods like Laplace's method[3].

¹The term *steepest descent* refers, for historical reasons, to the real part of *ig* (i.e. the negative imaginary part of *g*) which decreases fastest along a path of steepest descent. In literature the exponent is often $\omega v(x)$.

²Stationary points of g correspond to saddle points in the complex plane. This is the background for the term saddle points methods, a class of methods under which the method of steepest descent sorts.

The method of steepest descent requires complex analytic extensions of f and g. This requirement can however be relaxed e.g. to analyticity in appropriate parts of the complex plane. This follows from Cauchy's Theorem which requires analyticity only in the area encompassed by the integration path and the interval [a, b].



Figure 1.1: The analytic structure of the Airy-type oscillator $g(x) = x^3 - x/2$. Dashed lines mark the border between ridges(+) and valleys(-). Solid bold lines are paths of steepest descent from ± 1 and the stationary points

1.2 Numerical methods for oscillatory integrals

For classical quadrature methods there are several ways of characterising efficiency. Most of these, like the polynomial degree of precision, is a measure of how well integrals of smooth functions are approximated. For oscillatory quadrature we operate with a so-called *asymptotic order*. The asymptotic order gives the rate at which the error decreases with increasing ω , that means the leading order behaviour of the error of the method.

We say that the method $\mathcal{Q}[f]$ has order³ q if,

$$\mathcal{Q}[f] - \mathcal{I}[f] = \mathcal{O}(\omega^{-q}).$$

1.2.1 Filon-type methods

In the integral (1.1), if we replace the envelope function f with a polynomial p of order m, we get an approximation,

$$\mathcal{I}[f] \approx \mathcal{I}[p],$$

which can be obtained by a linear combination of moments $\mathcal{I}[x^j]$, j = 0, ..., m. In the case where the moments can be computed we are left with an interpolation problem. This is the basic idea behind Filon-type methods.

The key to analysing the efficiency of this approach is asymptotic expansions of the error. Here we limit the discussion to the case of no stationary points, and the relevant asymptotic expansion is (1.2). It can be proved with relative ease that the functions $\sigma_m[f]$, defined in (1.3), are of the form,

$$\sigma_m[f](x) = \sum_{j=0}^m \sigma_{m,j}(x) f^{(j)}(x), \qquad (1.7)$$

where $\sigma_{m,j}(x)$ only depend on g and its derivatives up to order m, evaluated in x. This implies the following lemma,

Lemma 1.1. Let f be an m times differentiable function such that $f^{(j)}(a) = f^{(j)}(b) = 0, j = 0, ..., m$. Assume $g'(x) \neq 0, x \in [a, b]$. Then,

$$\int_{a}^{b} f(x)e^{i\omega g(x)} \mathrm{d}x = \mathcal{O}(\omega^{-m-1}), \quad \omega \to \infty.$$

Proof. Considering the form of the functions $\sigma_m[f]$ in equation (1.7) it is clear that,

$$\sigma_j[f](a) = \sigma_j[f](b) = 0, \quad j = 0, \dots, m.$$

Combined with the asymptotic expansion (1.2) we get the desired conclusion. \Box

Now the asymptotic properties of Filon-type methods are easily obtained. From the linearity of the integration operation we get,

$$\mathcal{I}[f] - \mathcal{I}[p] = \mathcal{I}[f - p] = \mathcal{O}(\omega^{-m-1}),$$

³Note that this definition of asymptotic order is slightly misleading since the $\mathcal{I}[f] = \mathcal{O}(\omega^{1/r})$ itself, where r+1 is the order of the highest order stationary point in [a, b]. This is why some authors define the asymptotic order as the order of the relative error.

where m is the maximal number of derivatives of f that are interpolated by p at either of the endpoints a and b. That means the method is of asymptotic order m + 1. A similar argument employing the Iserles-Nørsett-expansion[16] shows that a method achieves order m if the polynomial p interpolates f and m - 1derivatives at regular endpoints, and $m \cdot (r_j + 1)$ derivatives at all q stationary points ξ_j of order r_j , $j = 1, \ldots, q$.

This clearly suggests that high asymptotic order can be achieved, in fact any asymptotic order, simply by using Hermite interpolation. Moreover, we can argue by referring to classical results in polynomial approximation that any tolerance can theoretically be achieved. Therefore we can get convergence, also for fixed ω . This as opposed to what asymptotic expansions can provide.

L.N.G. Filon's method from 1928[8] has not been confined to total obscurity, his article was cited quite regularly throughout the years. It is therefore a bit surprising that a proper analysis of the method came more than seventy years later. Interestingly, Filon did not identify the endpoints as critical, and suggested subdivision of the interval to obtain higher accuracy. In other words, Filon only considered the approximation properties of p with respect to f, and missed the perhaps more interesting asymptotic accuracy.

1.2.2 The numerical method of steepest descent

Considering the method of steepest descent, a quite simple observation with important implications is the fact that the *steepest-descent integral* (1.6) is of a form that is well suited for approximation by classical numerical methods. This will lead to methods with similar characteristics as those of the Filon-type methods.

First we make the following remark regarding the form of the paths of steepest descent.

Lemma 1.2. Assuming g is a complex analytic function at x. $h_x(p)$, any path of steepest descent originating at a point x is of the form

$$h_x(p) \sim x + a_1 p^{1/r} + a_2 p^{2/r} + \dots, \qquad p \to 0,$$

where r - 1 is the order of the stationary point if x is a stationary point, r = 1 otherwise.

Proof. For small p, $h_x(p) = x + \delta$, where δ is small. Being a complex analytic function, g has an expansion in integer powers where r - 1 terms drop out, therefore,

$$g(x+\delta) = g(x) + g_r \delta^r + g_{r+1} \delta^{r+1} + \dots$$

Inserting into equation (1.4) gives,

$$g_r\delta^r + g_{r+1}\delta^{r+1} + \ldots = ip,$$

An extension of the Lagrange-Bürmann formula(see Theorem 2.4f from [9]) provides that δ has r branches, each being complex analytic at p = 0 as a function of $p^{1/r}$. This concludes the proof.

It follows from this that the Jacobian of the path is not necessarily regular. However, with a change of variables $p \rightarrow q^r$, we get

$$\mathcal{I}[f,h_x] = r \int_0^\infty f(h_x(q^r)) h'_x(q^r) q^{r-1} e^{-\omega q^r} \mathrm{d}q,$$

which has an analytic integrand. A second change of variables $q \to t \omega^{-1/r}$ transforms the integral into a form where Gaussian quadrature with Freud-type weights e^{-t^r} can be applied. These are quadrature rules with nodes x_j and weights w_j ,

$$\sum_{j=1}^{n} w_j \varphi(x_j) \approx \int_0^\infty \varphi(t) e^{-t^r} \mathrm{d}t,$$

which are exact for $\varphi(t)$ being a polynomial of degree $\leq 2n-1$. Note that for r = 1 we have the well known Gauss-Laguerre rule, and the case r = 2 corresponds to half-space Hermite⁴.

In [6] it is proved that using this quadrature rule on the two steepest-descent integrals in equation (1.6) as here indicated yields a method Q[f] for which,

$$Q[f] - I[f] = \mathcal{O}(\omega^{-\frac{2n+1}{r}}),$$

where n is the number of quadrature points used on each of the integrals. Clearly, this approach provides approximations of high asymptotic order. In addition, it follows from the convergence properties of Gaussian quadrature that also the numerical method of steepest descent is actually convergent.

Filon-type methods and the numerical method of steepest descent are two very different approaches that yield efficient methods for oscillatory integrals, methods that can achieve high asymptotic order in ω while at the same time being convergent for fixed ω . These are however far from the only possibilities we have. Levin-type methods are based on a third approach which is quite different from the two approaches seen here. It is based on formulating the integral as a differential equation which can be solved e.g. by collocation or continuous GMRES[20, 27, 25].

⁴In the case where we use an incoming and outgoing path at a stationary point, it is beneficial to merge the two paths at a stationary point with r = 2 such that full Hermite quadrature may be applied. For higher r a similar observation holds, although for odd r the quadrature rules are slightly exotic[6].

1.3 High frequency scattering problems

Wave scattering problems appear in a large number of applications. The scattering of electromagnetic waves is important in antenna design, radar, fiber optics, MRI etc. Scattering of acoustic waves is central to sonar technology, seismic exploration, ultrasound imaging, architecture, and more. The applications are ubiquitous and appear as central in the engineering of many of the devices that stand as icons representing the contemporary world.

Techniques for high frequency asymptotics for scattering problems have a long history with incremental developments. The well known Geometric Optics approximation does good in many cases, but fail to deliver in special cases like diffraction, non-linear effects and intermediate frequencies. More sophisticated asymptotic techniques exist, but more and more effort is now being put into discretisation techniques. Recent developments has however given some very powerful hybrid approaches. These use both asymptotics and elements of discretisation techniques. Such approaches do a lot to increase the efficiency of solvers for scattering problems.

1.3.1 The Helmholtz equation

As a starting point for scattering problems we have the hyperbolic scalar wave equation

$$\frac{\partial^2 p}{\partial p^2} - c^2 \Delta p = 0, \qquad x \in D \subset \mathbb{R}^n.$$
(1.8)

This equation describes the propagation of waves in homogeneous media, n = 2, 3. A typical example is acoustic waves, in which case c is the speed of sound and p is the induced pressure. Electromagnetic waves can be expressed similarly with a vectorial version of the wave equation.

Time-harmonic solutions of (1.8) are functions of the form

$$p(x,t) = u(x)e^{-i\omega t},$$

where the function u(x) satisfies the elliptic Helmholtz equation, often referred to as the time-harmonic wave equation,

$$\Delta u + k^2 u = 0, \qquad x \in D \subset \mathbb{R}^n, \tag{1.9}$$

We call $k = \omega/c$ is the *wavenumber* of the problem. It is related frequency by the formula $f = kc/2\pi$.

The question of solvability of the Helmholtz equation must be treated differently for different geometries. In case the domain D is bounded, the Laplacian, with Dirichlet or Neumann boundary conditions, is self-adjoint. The Fredholm alternative then gives that either k^2 is not an eigenvalue of the Laplacian, and the problem is uniquely solvable, or k^2 is an eigenvalue, and eigenfunctions are solutions to (1.9). For an exterior problem, i.e. $D = \mathbb{R}^n \setminus \Omega$, where Ω is a bounded domain, an extra condition at infinity is needed in order for the solution to be uniquely solvable. This is the Sommerfeld radiation condition which makes sure that the solution is outgoing at infinity, thereby eliminating unphysical solutions. A common expression for the condition is,

$$\left|\frac{\partial u^s}{\partial r} - iku^s\right| \le \frac{c}{r^2}, \quad r \to \infty.$$

The Helmholtz equation (1.9) in free space possesses two solutions that are of particular interest. The first is a plane wave traveling in the direction d,

$$u(\mathbf{x}) = e^{ik\mathbf{d}^T\mathbf{x}}, \qquad |\mathbf{d}| = 1.$$

The plane wave does not satisfy the radiation condition. It is however still of great use since, for example, it can be used as a model for point sources at large distances. The second solution of interest to us is the fundamental solution or Greens function, i.e. the solution to the problem with a point source at the origin,

$$\Delta G + k^2 G = -\delta_0$$

 δ_0 is the Dirac delta at the origin, and the radiation condition is imposed . The fundamental solution for n=2 is

$$G(r) = -\frac{1}{4i}H_0^{(1)}(kr), \qquad (1.10)$$

with $H_0^{(1)}$ being the order zero Hankel function of the first kind. In the case n = 3 the fundamental solution is,

$$G(r) = \frac{1}{4\pi r} e^{ikr} \tag{1.11}$$

1.3.2 Problem formulation

Consider an obstacle Ω which is a bounded domain of space \mathbb{R}^n . We shall consider solutions to (1.9) in the exterior of the obstacle, $\mathbb{R}^n \setminus \Omega$. Necessary boundary conditions on Γ , the surface of Ω , are imposed by modelling. They can be of Dirichlet-type $u|_{\Gamma} = g_D$, Neumann-type $\frac{\partial u}{\partial n}|_{\Gamma} = g_N$ or combinations thereof.

In the following we shall assume that Ω is smooth and strictly convex, and also, for simplicity, we assume a perfectly reflecting boundary conditions, i.e. a

zero Dirichlet condition $g_D = 0$. This last assumption on the boundary condition is not crucial; general boundary conditions yield problems with similar characteristics. It turns out, however, that the smoothness and convexity of Ω is an assumption with deeper consequences. Sharp corners on Ω give rise to diffraction phenomena that are fundamentally different from reflections. Non-convex scatterers may exhibit multiple reflections which among other things destroy asymptotic localization properties.

The scattering problem concerns finding the scattered field u^s given an incoming field u^i , both satisfying (1.9), with boundary conditions imposed on the total field $u = u^s + u^i$, and the radiation condition imposed on the scattered field,

$$\Delta u^{s} + k^{2}u^{s} = 0, \quad x \in \mathbb{R}^{n} \setminus \Omega,$$

$$u^{s} = -u^{i}, \quad x \in \Gamma$$

$$\left|\frac{\partial u^{s}}{\partial r} - iku^{s}\right| \leq \frac{c}{r^{2}} \quad r \to \infty.$$
(1.12)

The last equation here is the radiation condition, and with it this problem is indeed well-posed[23].

1.3.3 Asymptotics of the highly oscillatory scattering problem



Figure 1.2: Illustration of the asymptotics of a smooth convex scatterer with an incident plane wave. In the illuminated region (1) waves behave according to Geometric Optics. In the Foch-Leontovič-regions (2 and 3) Geometric Optics break down. The field in the shadow region (4) is due to diffraction phenomena

For the high frequency behaviour of solutions to the scattering problem (1.12) it is natural to try a WKB-type ansatz of the form,

$$u^{s}(\mathbf{x}) \sim \sum_{j=0}^{\infty} \frac{A_{j}(\mathbf{x})}{(ik)^{j}} e^{iku(\mathbf{x})}, \qquad k \to \infty.$$

This leads to the well known eikonal and transport equations,

$$(\nabla u)^2 = 1,$$
 (1.13)

$$A_j \nabla u + 2\nabla A_j \nabla u = -\Delta A_{j-1}, \quad j = 0, 1, \dots$$
(1.14)

Here $A_{-1} = 0$ by convention. The eikonal equation (1.13) can presumably be solved by the method of characteristics, giving the rays known from Geometric Optics. The leading order transport equation can also be solved explicitly. Together this means that the leading order of the reflected field can be computed explicitly[29]. Although this approach seems promising, it's only the beginning of a very long story. In case the obstacle under consideration is non-convex, *caustics* may appear, i.e. the field at a point may be determined by more than one ray, and the approximation is no longer valid. Note that we exclude this case by assumption. Otherwise, when approaching a point of ray tangency, a point on the boundary between the illuminated part of the obstacle and shadow, the series break down. Also the series will be insufficient to predict the small but non-zero solution in the shadow. This means fore example that diffraction effects are unaccounted for.

Near the point of ray tangency a special asymptotic region can be identified. This region, known as the Fock-Leontovič region, has a size that scales with $k^{-1/3}$ to either side of the tangency point along the surface, and $k^{-2/3}$ normal to the surface. The leading order is here given by the Fock-Leontovič equation[19].

In the shadow region the failure of the WKB-type ansatz reflects the *extra* polynomial decay of the solution. In other words the wave field vanishes faster than any inverse power of k in the shadow. Still, a number of interesting phenomena play out in the shadow. For example will we have that the surface itself is a caustic of the eikonal equation. Rays tangent to the surface will diffract and follow the surface while at the same time shedding rays tangentially. Such solutions decay quickly. However, these *creeping rays* are important in applications[22].

The connection of the behaviours at the different regions is a highly non-trivial problem of uniform asymptotics. A solution does exist in a paper by Melrose and Taylor[21]. These results have yet to be applied in computations.

1.3.4 Integral equation representations

The scattering problem can be formulated as an integral equation over Γ , the surface of the scatterer Ω . This is done through the layer potentials. The *single layer potential* is written,

$$u^{s}(y) = (Sq)(y) := \int_{\Gamma} G(x-y)q(x)\mathrm{d}S_{x},$$

and the double layer potential,

$$u^{s}(y) = (D\varphi)(y) := \int_{\Gamma} \frac{\partial G}{\partial n_{x}}(x-y)\varphi(x) \mathrm{d}S_{x}.$$

q and φ are defined on Γ and are usually referred to as the single and double layer potential densities.

The layer potentials automatically satisfy the radiation condition, and they solve the Helmholtz problem both in the exterior and interior of Ω . It is shown e.g. in [23], that the single layer potential is continuous in y, while its normal derivative is discontinuous when crossing Γ . Similarly the double layer potential has a continuous normal derivative, but is itself discontinuous when crossing Γ . From this it follows that u solves both the exterior and interior Dirichlet problem if q solves,

$$(Sq)(y) = -u^{i}(y), \qquad y \in \Gamma.$$

The discontinuous double layer potential density φ solves,

$$\left(\left(\frac{I}{2}+D\right)\varphi\right)(y) = -u^i(y), \qquad y \in \Gamma,$$

if u is to solve the exterior Dirichlet problem, and

$$\left(\left(-\frac{I}{2}+D\right)\varphi\right)(y) = -u^{i}(y), \qquad y \in \Gamma,$$

for the interior problem. Similar relations exist for the Neumann problem[23].

The tight connection between the interior and exterior problems poses a particular problem. If we wish to solve the exterior problem, we solve the interior problem at the same time, which is, as pointed out above, not necessarily uniquely solvable. In this case the operators are not invertible. However, a trick due to Brakhage and Werner[4] is to use an operator,

$$u^{s}(y) = (i\alpha S(q) - D(q))(y).$$

This operator is invertible for all k provided α is real.

1.3.5 Numerical methods for high frequency scattering problems

By a numerical method for high frequency scattering problems we mean a method that in some way incorporates the high frequency asymptotics of the solution. The goal of this would be to develop methods whose computational effort is bounded or decreasing as $k \to \infty$ while maintaining constant precision, also for moderate wavenumbers.

One approach that goes a long way in achieving this, at least for convex obstacles, is by the use of boundary elements where asymptotic properties of the solution are incorporated[5]. Other approaches include the use of fast multipole methods or hierarchical matrices(see [10] for a review of such techniques).



Discretisation based on oscillatory quadrature

Figure 1.3: The absolute value of the real and imaginary parts of the single layer potential density q for a circle with an incident plane wave. (b) shows q with the GO-phase factored out. Bold lines marks position of shadow boundaries

Ignoring for the time being possible difficulties of non-uniqueness, an integral equation for the single layer potential density written out for the case n = 2 is

$$-\frac{1}{4i} \int_{\Gamma} H_0^{(1)}(k|x-y|)q(x) \mathrm{d}s_x = -u^i(y).$$

For the Hankel function the behaviour for large arguments is,

$$H_0^{(1)}(r) \sim \sqrt{\frac{2}{\pi r}} e^{i(r-1/4\pi)}.$$

The oscillatory behaviour for large arguments e^{ir} can be factored, out and the remainder is non-oscillatory. Similarly, the density q is oscillatory, but here we can use high frequency asymptotics, e.g. Geometric Optics, to factor out the oscillatory part. The Geometric Optics approximation, which is valid in the illuminated part of a smooth obstacle gives,

$$q(x) = q_s(x)e^{ikg_i(x)}$$

where q_s is smooth and g_i is the phase of the incoming wave. After this *phase* extraction we have an equation of the form,

$$\int_{\Gamma} K(x,y)q_s(x)e^{ik(|x-y|+g_i(x))} \mathrm{d}s_x = -u^i(y).$$
(1.15)

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where $K(x, y) = \frac{i}{4}H_0^{(1)}(k|x - y|)e^{-k|x-y|}$ is a smooth function. q_s can only be expected to be smooth wherever the Geometric Optics approximation is valid, thus q_s can be expected to be oscillatory in the shadow region, which indeed can be seen in Figure 1.3. Boundary element discretisations based on this formulation of the problem are of great interest since one solves for a field that is less oscillatory than q, the unknown in the standard formulation. Such hybrid approaches are proved to require only a moderate increase in unknowns with increasing k for fixed error bounds $(n \sim k^{1/9} \text{ in } [7].)$

The kernel of the integral operator (1.15) is oscillatory, and a discretisation has to take this into account. A Filon-type discretisation is done by first identifying contributing points. By examining the oscillator $|x - y| + g_i(x)$ we get that the only stationary points are to be found in the shadow region[2]. Since the solution is both oscillatory and exponentially small in the shadow region[7] we can neglect these contributions bearing in mind that they might not be negligible in moderate wavenumber regimes. We are left with a contribution from a discontinuous derivative combined with the logarithmic singularity of $H_0^{(1)}(k|x - y|)$ at x = y. The moments of this Filon-quadrature are oscillatory quadratures themselves, but these can be computed efficiently with the numerical method of steepest descent. This, coupled with a special treatment of the Fock-Leontovič regions and shadow region gives a method that has at least fixed accuracy for increasing k[13].

1.4 Summary of the main contribution of the thesis

The work leading to this thesis has revolved around the application of oscillatory quadrature methods to practical problems. The most important case study has been the acoustic scattering from a smooth convex obstacle. For this problem, a discretisation technique due to Huybrechs and Vandewalle[13] employs both the Filon-type approach and numerical steepest descent. One of the main contributions of this thesis has been a more thorough treatment of this method. Notably, a reinterpretation of the method shows that it can be regarded as a method for obtaining the near-equivalent of high order Geometric Optics approximations. This work also paves the way for more sophisticated discretisations based on the uniform asymptotics of Melrose and Taylor.

An important element in the implementation of the Filon-type discretisation is the computation of the moments. This is done by the numerical method of steepest descent. A difficulty here is the computation of the paths of steepest descent, which has been an issue in this work. One of the contributions here is the analysis of the numerical method of steepest descent with local path approximations, which shows exactly how asymptotic accuracy deteriorates when paths are approximated.

A final theme, which resulted in the first paper of this thesis, is the basis of oscillatory quadrature and asymptotics. Asymptotic expansions can be expressed with an exact error term. An alternative approach to oscillatory quadrature, similar to techniques in hyperasymptotics, is to resolve the error term by oscillatory quadrature. This leads to new methods with new characteristics.

1.4.1 Summary of papers

Paper I: A combined Filon/Asymptotic quadrature method for highly oscillatory problems

A. Asheim Published in BIT Numerical Mathematics 48, 2008[1]

This paper discusses a combination of asymptotic expansions and Filon-type methods. An asymptotic expansion has a remainder term that can be expressed as an oscillatory integral. Resolving this oscillatory integral with e.g. a Filon-type method yields a new type of approximation that combines properties of both constituent methods. A discussion on possible gains from using this approach is included, which concludes that in certain cases significant savings in terms of moments can be achieved.

Paper II:Asymptotic analysis of numerical steepest descent with path approximations

A. Asheim and D. Huybrechs To appear in Found. Comput. Math.

A difficulty with steepest descent methods lies in the computation of the paths of steepest descent. It is however well known from asymptotics that a certain slack can be tolerated. In this paper we translate this observation into the numerical setting. A central difference between the numerical and asymptotic setting is the more localised character of the numerical method; the form of the path for large arguments is in some sense irrelevant. It is shown that a local approximation of the path is sufficient for high asymptotic order, and the main part of the paper analyses the asymptotic properties of the method. The result is a slightly unintuitive relation between the degree of the path approximation and the method's order.

Paper III: Local solutions to high frequency scattering problems

A. Asheim and D. Huybrechs To appear in J.Comput.Phys.

Classical asymptotic techniques show that the scattering from convex bodies depends on local characteristic, meaning that an incident ray is reflected according to the properties of the scatterer only where it strikes. In this paper we show that a Filon-type discretisation transforms the boundary integral equation for the scattering problem to a boundary value problem for a differential equation. This equation can be solved with local data only to give a high order approximation, which corresponds to the localisation principle known from Geometric Optics.

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Paper I

A combined Filon/Asymptotic quadrature method for highly oscillatory problems

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Chapter 2

A combined Filon/Asymptotic quadrature method for highly oscillatory problems

Abstract. A cross between the asymptotic expansion of an oscillatory integral and the Filon-type methods is obtained by applying a Filon-type method on the error term in the asymptotic expansion, which is in itself an oscillatory integral. The efficiency of the approach is investigated through analysis and numerical experiments, revealing a method which in many cases performs better than the Filon-type method. It is shown that considerable savings in terms of the required number of potentially expensive moments can be expected. The case of multivariate oscillatory integrals is discussed briefly.

2.1 Introduction

The quadrature of highly oscillatory integrals has been perceived as a hard problem. Traditionally one would have to resolve the oscillations by taking several sub-intervals for each period, resulting in a scheme whose complexity would grow linearly with the frequency of the oscillations. More careful analysis will however reveal that by exploiting the structure of certain classes of oscillatory integrals better discretisation schemes can be devised, schemes where the error actually decreases when the frequency of the oscillations increases. This is well known in asymptotic analysis with eg. saddle point methods and the method of stationary phase approximation[16, 14]. Recently attention has been directed at numerical methods with similar properties. Examples of such methods are Filon-type methods[8, 9] Levin-type methods[13, 15] and numerical steepest descent[6].

We are considering oscillatory integrals of the form

$$I[f] = \int_{-1}^{1} f(x)e^{i\omega g(x)} \mathrm{d}x,$$
(2.1)

where ω is a large parameter. It is well known that an ordinary Gaussian quadrature applied to this integral will have an error of $\mathcal{O}(1)$ as ω grows large. A much better approach to approximating I[f] when ω is large is found through an asymptotic expansion: Assuming $g'(x) \neq 0, -1 \leq x \leq 1$, integration by parts yields

$$I[f] = \frac{1}{i\omega} \left[\frac{f(1)}{g'(1)} e^{i\omega g(1)} - \frac{f(-1)}{g'(-1)} e^{i\omega g(-1)}\right] - \frac{1}{i\omega} \int_{-1}^{1} \frac{\mathrm{d}}{\mathrm{d}x} \left[\frac{f(x)}{g'(x)}\right] e^{i\omega g(x)} \mathrm{d}x.$$
 (2.2)

When ω becomes large the integral term in equation (2.2) vanishes faster than the boundary terms, by an extension of Riemann-Lebesgue's lemma, so the boundary terms can approximate the integral. Furthermore the process can be repeated on the integral remainder to obtain a full asymptotic expansion. This expansion will however not be perfect. As is often the case with asymptotic expansions the accuracy is limited due to the divergence of the series.

An even better approach is to choose a set of quadrature nodes c_1, \ldots, c_{ν} , interpolate the function f by a polynomial \tilde{f} at these points and let

$$Q_1^F[f] = \int_{-1}^1 \tilde{f}(x) e^{i\omega g(x)} dx = \sum_{j=1}^{\nu} b_j(\omega) f(c_j),$$

where $b_j(\omega) = \int_{-1}^{1} l_j(x)e^{i\omega g(x)} dx$ for $l_j(x)$ the *j*-th Lagrange cardinal polynomial. A variant of this approach, then with piecewise quadratic interpolation in the Fourier-case when g(x) = x, dates back to L.N.G. Filon[4]. Schemes of this type are referred to as Filon-type methods. Constructing $b_j(\omega)$ requires the moments

 $\int_{-1}^{1} x^m e^{i\omega g(x)} dx$. Moments are oscillatory integrals themselves that hopefully can be calculated by analytical means as in the Fourier case. If not, the numerical steepest descent method can be applied to compute moments for the Filon-type method, an approach which works well in practical applications[7, 2]. Iserles proved[8] that as long as the endpoints of the interval are included as quadrature nodes and $g'(x) \neq 0, -1 \leq x \leq 1$, this approach will carry an error

$$Q_1^F[f] - I[f] \sim \mathcal{O}(\omega^{-2}), \quad \omega \to \infty.$$

The superiority of this approach over the asymptotic expansion can be understood by realising that the method is exact for a class of problems, regardless of the size of ω . As for the behaviour for large ω it was proved by Iserles and Nørsett[11] that by applying Hermite interpolation to interpolate f(x) with p derivatives at the endpoints, the asymptotic behaviour of the error can be expressed as

$$Q_p^F[f] - I[f] \sim \mathcal{O}(\omega^{-p-1}), \quad \omega \to \infty.$$

The theory can be expanded to the cases where g has stationary points, that means points ξ with $g'(\xi) = 0$. What must be done to achieve good asymptotic properties is basically to include the stationary points among the quadrature nodes[9].

Considering the asymptotic expansion with the remainder term (2.2) one cannot fail to notice that the problem has really been transformed into boundary terms plus the remainder term, which is an integral of the same form as the original. A natural question to ask in light of this observation is whether treating the remainder term with a specialised technique, like the Filon-type quadrature, numerical steepest descent or a Levin-type method, could improve accuracy. In the following this question will be addressed, in particular for the choice of the Filon-type quadrature Q_p^F as quadrature method. In the above-mentioned case this would amount to a new method

$$Q^{FA}[f] = \frac{1}{i\omega} \left[\frac{f(1)}{g'(1)} e^{i\omega g(1)} - \frac{f(-1)}{g'(-1)} e^{i\omega g(-1)} \right] - \frac{1}{i\omega} Q_p^F \left[\frac{\mathrm{d}}{\mathrm{d}x} [f/g'] \right].$$

We will refer to methods of this form as *combined Filon/asymptotic methods*. Observe that for $\omega \neq 0$ this method is consistent in the sense that accuracy can be improved by using a better quadrature method on the remainder term, a property which the asymptotic expansion does not have. Furthermore, because of the $1/\omega$ -factor, the asymptotic error behaviour will be better than for the classical Filon-type method applied directly. This means that less work, in terms of moments, is needed to get high asymptotic order. The combined method is in this sense a true cross between the asymptotic method and the Filon-type method, combining

good qualities of both methods. These observations will be elaborated on in the following with emphasis on the 1D case without stationary points, with stationary points and a brief look into the multivariate case.

2.2 The Asymptotic method and Filon-type methods

We begin the exposition by presenting an overview of the constituent parts of the combined method: The asymptotic expansion of the highly oscillatory integral and the Filon-type methods. In the following we will denote by $Q_p[f] \approx I[f]$ a highly oscillatory quadrature method of *asymptotic order p*, meaning that for smooth f

$$Q_p[f] - I[f] \sim \mathcal{O}(\omega^{-p-1}), \quad \omega \to \infty.$$

Note that in some parts of the literature this would be referred to as order p + 1. This corresponds to absolute error decay, whereas ours is relative error decay in the case of no stationary points where $I[f] \sim 1/\omega$ [16]. In the presence of stationary points the picture is slightly different, and for simplicity we will then avoid the concept of asymptotic order.

2.2.1 The case of no stationary points

Assume for the time being that there are no stationary points in the interval of interest, that means $g'(x) \neq 0$, $-1 \leq x \leq 1$. An asymptotic expansion of the highly oscillatory integral (3.1) is obtained by successively applying integration by parts. This approach gives us a full expansion through the following partial expansion

$$I[f] = -\sum_{m=1}^{s} \frac{1}{(-i\omega)^m} \left[\frac{e^{i\omega g(1)}}{g'(1)} \sigma_{m-1}[f](1) - \frac{e^{i\omega g(-1)}}{g'(-1)} \sigma_{m-1}[f](-1) \right] + \frac{1}{(-i\omega)^s} \int_{-1}^{1} \sigma_s[f](x) e^{i\omega g(x)} \mathrm{d}x,$$
(2.3)

where

$$\sigma_0[f](x) = f(x) \sigma_{m+1}[f](x) = \frac{d}{dx} \frac{\sigma_m[f](x)}{g'(x)}, \quad k = 0, 1, \dots$$
(2.4)

The correctness of the above expansion can easily be checked through an induction argument. A full asymptotic expansion of the highly oscillatory integral (3.1) is

then

$$I[f] \sim -\sum_{m=1}^{\infty} \frac{1}{(-i\omega)^m} \left[\frac{e^{i\omega g(1)}}{g'(1)} \sigma_{m-1}[f](1) - \frac{e^{i\omega g(-1)}}{g'(-1)} \sigma_{m-1}[f](-1) \right].$$
(2.5)

Truncating the series after s terms, yields the asymptotic method

$$Q_s^A[f] = -\sum_{m=1}^s \frac{1}{(-i\omega)^m} \left[\frac{e^{i\omega g(1)}}{g'(1)} \sigma_{m-1}[f](1) - \frac{e^{i\omega g(-1)}}{g'(-1)} \sigma_{m-1}[f](-1) \right].$$
(2.6)

The method has asymptotic order s. This can be seen by writing out the remainder term, which is an oscillatory integral $\mathcal{O}(\omega^{-1})$ multiplied by $(-i\omega)^{-s}$. Note that the concept of asymptotic order is rather useless for not-so-large ω . In fact the asymptotic expansion is divergent in the general case, and this divergence is more severe for smaller ω . Thus the asymptotic method is rather useless for small ω . Furthermore, divergence implies that only a fixed accuracy can be attained adding terms will not always increase accuracy. This is problematic for practical applications where usually a given accuracy is sought.

The Filon-type methods will be accurate also for smaller ω and have controllable error, but that is at the cost of moments. We define the moments

$$\mu_k(\omega) = \int_{-1}^1 x^k e^{i\omega g(x)} \mathrm{d}x,$$

and assume these can be computed, possibly at a significant cost. Then the Filontype method is obtained by choosing a set of nodes $-1 = c_1 < c_2 < \cdots < c_{\nu} = 1$ and integer multiplicities $m_1, \ldots, m_{\nu} \ge 1$ associated with each node. Let $n = \sum_{j=1}^{\nu} m_j - 1$ and \tilde{f} be the unique Hermite interpolation polynomial of degree *n* obtained by interpolating *f* at the points $\{c_j\}_{j=1}^{\nu}$ with the corresponding multiplicities,

$$\tilde{f}(x) = \sum_{l=1}^{\nu} \sum_{j=0}^{m_l-1} \alpha_{l,j}(x) f^{(j)}(c_l).$$

The Filon-type method is defined as

$$Q_s^F[f] = \int_{-1}^1 \tilde{f}(x) e^{i\omega g(x)} dx = \sum_{l=1}^{\nu} \sum_{j=0}^{m_l-1} \beta_{l,j}(\omega) f^{(j)}(c_l),$$
(2.7)

where $\beta_{l,j}(\omega) = \int_{-1}^{1} \alpha_{l,j}(x) e^{i\omega g(x)} dx$ is obtained from linear combinations of moments. As for *s*, the asymptotic order of this method, we state a theorem due to Iserles and Nørsett[11]:

Theorem 2.1. Suppose $m_1, m_\nu \ge s$, then for every smooth f and smooth g with $g'(x) \ne 0, -1 \le x \le 1$

$$Q_s^F[f] - I[f] \sim (\omega^{-s-1}), \quad \omega \to \infty.$$

The proof is obtained by expanding $f - \tilde{f}$ as in equation (2.5) and observing that the first s terms will cancel due to the interpolation criteria. This theorem can be summarised by saying that only by adding derivative information at the endpoints of the interval can the asymptotic order of the method be improved. Information about derivatives can also be supplied indirectly by clustering interpolation nodes near the endpoints. If the nodes approach the endpoints as $1/\omega$ high asymptotic order can be attained[10]. Note that increasing the order of the interpolating polynomial \tilde{f} will increase the accuracy of the method for some fixed ω , at least when the interpolation nodes are the Chebychev points. This is indeed confirmed by numerical experiments[10]. This means that for any ω a prescribed accuracy can be attained, a property which is crucial for practical applications.

2.2.2 Generalized Filon and asymptotic method in the presence of stationary points

When g has stationary points Theorem 2.1 is no longer valid, a fact which is suggested by the singularity introduced in the integral in remainder term of the asymptotic expansion (2.2). Assume in the following that g(x) has only one stationary point $\xi \in (-1, 1)$, which amounts to saying $g'(\xi) = 0$, $g'(x) \neq 0, x \in [-1, 1] \setminus \{\xi\}$. Furthermore assume that $g'(\xi) = \cdots = g^{(r)}(\xi) = 0$, and $g^{(r+1)}(\xi) \neq 0$, this means that ξ is a *r*th order stationary point. The method of stationary phase[3, 14] states that in this case the leading order behaviour of the highly oscillatory integral (3.1) is of the form

$$I[f] \sim C\omega^{-1/(r+1)}, \quad \omega \to \infty.$$
 (2.8)

This means that the main contribution to the value of the integral comes from the stationary point, suggesting that the interpolation nodes for the Filon-type methods should include stationary points as well as the endpoints.

Assume for simplicity that ξ is a first order stationary point meaning $g'(\xi) = 0$ and $g''(\xi) \neq 0$. Writing

$$\begin{split} I[f] &= f(\xi)I[1] + I[f - f(\xi)] \\ &= f(\xi)I[1] + \frac{1}{i\omega} \int_{1}^{-1} \frac{f(x) - f(\xi)}{g'(x)} \frac{\mathrm{d}}{\mathrm{d}x} e^{i\omega g(x)} \mathrm{d}x, \end{split}$$
then integrating by parts gives the following expression:

$$I[f] = f(\xi)I[1] + \frac{1}{i\omega} \left[\frac{f(1) - f(\xi)}{g'(1)} e^{i\omega g(1)} - \frac{f(-1) - f(\xi)}{g'(-1)} e^{i\omega g(-1)} \right] - \frac{1}{i\omega} \int_{-1}^{1} \frac{\mathrm{d}}{\mathrm{d}x} \frac{f(x) - f(\xi)}{g'(x)} e^{i\omega g(x)} \mathrm{d}x.$$
(2.9)

Now, since $g''(\xi) \neq 0$, the singularity is removable. The expansion can be continued giving a full expansion reminiscent of the expansion (2.5). More generally, for a *r*th order stationary point we introduce the generalized moments

$$\mu_k(\omega;\xi) = I[(\cdot - \xi)^k] = \int_{-1}^1 (x - \xi)^k e^{i\omega g(x)} dx, \quad k \ge 0$$

Note that these can be written in terms of ordinary moments. Now write

$$I[f] = \sum_{j=0}^{r-1} \frac{1}{j!} f^{(j)}(\xi) \mu_j(\omega;\xi) + I\left[f(x) - \sum_{j=0}^{r-1} \frac{1}{j!} f^{(j)}(\xi) (x-\xi)^j\right].$$
 (2.10)

Again the singularity is removable, and the expansion can be formed. We will later need the expansion with the remainder term, so this will be formulated as a lemma¹:

Lemma 2.1. Suppose ξ is a stationary point of order r, and that ξ is the only stationary point inside the interval [-1, 1]. Then for every smooth f

¹Note that the conclusion in this lemma is different from that of Iserles & Nørsett in [11], Theorem 3.2, which we suggest is flawed.

where

$$\rho_0[f](x) = f(x)$$

$$\rho_{m+1}[f](x) = \frac{\mathrm{d}}{\mathrm{d}x} \frac{\rho_m[f](x) - \sum_{j=0}^{r-1} \frac{1}{j!} \rho_m[f]^{(j)}(\xi)(x-\xi)^j}{g'(x)}.$$
(2.12)

Proof. This is proved by induction. The Lemma is certainly true for s = 0. Now

$$I\left[\rho_{s}[f]\right] = \sum_{j=0}^{r-1} \frac{1}{j!} \rho_{s}[f]^{(j)}(\xi) \mu_{j}(\omega;\xi) + \frac{1}{i\omega} \int_{-1}^{1} \frac{\rho_{s}[f](x) - \sum_{j=0}^{r-1} \frac{1}{j!} \rho_{s}[f]^{(j)}(\xi)(x-\xi)^{j}}{g'(x)} \frac{\mathrm{d}}{\mathrm{d}x} e^{i\omega g(x)} \mathrm{d}x.$$

Integration by parts gives

$$\begin{split} I\Big[\rho_s[f]\Big] &= \sum_{j=0}^{r-1} \frac{1}{j!} \rho_s[f]^{(j)}(\xi) \mu_j(\omega;\xi) \\ &\quad - \frac{1}{(-i\omega)} \Bigg[\frac{e^{i\omega g(1)}}{g'(1)} \Big(\rho_s[f](1) - \sum_{j=0}^{r-1} \frac{1}{j!} \rho_s[f]^{(j)}(\xi)(1-\xi)^j\Big) \\ &\quad - \frac{e^{i\omega g(-1)}}{g'(-1)} \Big(\rho_s[f](-1) - \sum_{j=0}^{r-1} \frac{1}{j!} \rho_s[f]^{(j)}(\xi)(-1-\xi)^j\Big) \Bigg] \\ &\quad + \frac{1}{(-i\omega)} I\Big[\rho_{s+1}[f]\Big]. \end{split}$$

Inserting into equation (2.11) proves the Lemma.

 \square

As before, truncating the expansion (2.11), that is the two *m*-summations after *s* terms, yields the asymptotic method. The asymptotic behaviour of the error in this method is found by the method of stationary phase applied to the remainder. Thus we get for the asymptotic method,

$$Q^{A}[f] - I[f] \sim \mathcal{O}(\omega^{-s-1/(r+1)}), \quad \omega \to \infty.$$

For an even more general case, in the presence of more than one stationary point, the interval can be partitioned such that each sub interval contains only one stationary point, and then an expansion can be made for each sub interval. As before, truncating the expansion after s terms yields the asymptotic method.

Now to the Filon-type method: Let ξ be a unique stationary point of order $r: g'(\xi) = 0$ and $g'(x) \neq 0$ for $x \in [-1,1] \setminus \{\xi\}, g'(\xi) = \cdots = g^{(r)}(\xi) = 0$, and $g^{(r+1)}(\xi) \neq 0$. The generalized Filon method[11] is constructed by choosing nodes $-1 = c_1 < c_2 < \cdots < c_{\nu} = 1$ such that the stationary point is among the nodes, that is $c_q = \xi$ for some $q \in \{1, 2, \dots, \nu\}$. Given multiplicities $m_1, m_2, \dots, m_{\nu} \geq 1$ corresponding to each node, we let \tilde{f} be the unique Hermite interpolation polynomial of degree $n = \sum_{j=1}^{\nu} m_j - 1$ obtained by interpolating f at the points $\{c_j\}_{j=1}^{\nu}$ with the corresponding multiplicities. The method is now simply

$$Q^F[f] = \int_{-1}^1 \tilde{f}(x) e^{i\omega g(x)} \mathrm{d}x.$$

The above integral is computed from linear combinations of moments.

We present another theorem by Iserles and Nørsett[11] regarding the asymptotic error behaviour of the generalized Filon method.

Theorem 2.2. Let $m_1, m_\nu \ge s$ and $m_q \ge s(r+1) - 1$. Then

$$Q^F[f] - I[f] \sim \mathcal{O}(\omega^{-s-1/(r+1)}), \quad \omega \to \infty.$$

This theorem is, like Theorem 2.1 proved by expanding $f - \tilde{f}$ and showing that terms up to order *s* cancel. The method is trivially expanded to cater for several stationary points, possibly of different order.

2.3 The combined Filon/asymptotic method

Let us for the moment assume that there are no stationary points of g in [-1, 1]. This assumption will be relaxed later on. A combined Filon/asymptotic method is constructed from the asymptotic expansion with the remainder term (2.3) by applying a Filon-type method on the remainder term, which is in itself an oscillatory integral. Denoting by $Q_{p,s}^{FA}$ a method which is obtained by applying a p-th order Filon-type method on the remainder of an s-term expansion we get

$$Q_{p,s}^{FA}[f] = -\sum_{m=1}^{s} \frac{1}{(-i\omega)^m} \left[\frac{e^{i\omega g(1)}}{g'(1)} \sigma_{m-1}[f](1) - \frac{e^{i\omega g(-1)}}{g'(-1)} \sigma_{m-1}[f](-1) \right] + \frac{1}{(-i\omega)^s} Q_p^F[\sigma_s[f]],$$
(2.13)

where the $\sigma_m[f]$ are defined as in equation (2.4). Note that this formula is consistent for $\omega \neq 0$ in the sense that if we resolve the remainder term exactly, then the formula is exact as well. Furthermore, note that the idea is not restricted to Filon-type methods. Any quadrature method Q_p can be applied:

Theorem 2.3. Let g be such that $g'(x) \neq 0, -1 \leq x \leq 1$. Applying a highly oscillatory quadrature method Q_p of asymptotic order p on the remainder in the s-term asymptotic expansion (2.3) yields a method $Q_{p,s}$. Applied to any smooth f this method is of order p + s, that is

$$Q_{p,s}[f] - I[f] \sim \mathcal{O}(\omega^{-p-s-1}), \quad \omega \to \infty.$$

Proof. Writing out the asymptotic expansion of $Q_{p,s}[f] - I[f]$ gives

$$\begin{aligned} Q_{p,s}[f] - I[f] &\sim \frac{1}{(-i\omega)^s} Q_p[\sigma_s[f](x)] \\ &+ \sum_{m=s+1}^{\infty} \frac{1}{(i\omega)^m} \left[\frac{e^{i\omega g(1)}}{g'(1)} \sigma_{m-1}[f](1) - \frac{e^{i\omega g(-1)}}{g'(-1)} \sigma_{m-1}[f](-1) \right] \\ &= \frac{1}{(-i\omega)^s} \left(Q_p[\sigma_s[f](x)] - \sum_{j=1}^{\infty} \frac{1}{(i\omega)^j} \left[\frac{e^{i\omega g(1)}}{g'(1)} \sigma_{j-1}[\sigma_s[f]](1) \right. \\ &\left. - \frac{e^{i\omega g(-1)}}{g'(-1)} \sigma_{j-1}[\sigma_s[f]](-1) \right] \right) \\ &\sim \frac{1}{(-i\omega)^s} \mathcal{O}(\omega^{-p-1}) = \mathcal{O}(\omega^{-p-s-1}), \end{aligned}$$

where the last line appears by using the asymptotic error property of the method Q_p .

We will here limit our attention to the case where Q_p is a Filon-type method, and we call the combined method $Q_{p,s}^{FA}$ a Filon/asymptotic method.

Example 2.1. For the simplest case set s = 1 and get

$$Q_{p,1}^{FA}[f] = \frac{1}{i\omega} \left[\frac{e^{i\omega g(1)}}{g'(1)} f(1) - \frac{e^{i\omega g(-1)}}{g'(-1)} f(-1) \right] - \frac{1}{i\omega} Q_p^F \left[\frac{\mathrm{d}}{\mathrm{d}x} \frac{f}{g'} \right], \quad (2.14)$$

which is a method of asymptotic order p + 1.

Example 2.2. We wish to compute

$$\int_{-1}^{1} \frac{e^{i\omega x}}{2+x} \mathrm{d}x.$$

Interpolating f(x) = 1/(2 + x) and its first derivative at x = -1 and x = 1 will give us a Filon-type method of asymptotic order s = 2. This method requires



Figure 2.1: The absolute value of the error for the combined Filon/asymptotic method (top) and the classical Filon-type method (bottom) from example 2.2, all scaled by ω^3

four moments. Interpolating only the function value of $\sigma_1(x) = -1/(2+x)^2$ at the two endpoints gives the combined Filon/asymptotic scheme which is also of asymptotic order 2, but only needs two moments. We expect this to be at the cost of not that good approximation properties compared to the classical method, which is indeed confirmed by experiments, see figure 2.1. Note that the crests of the curve of one method seems to correspond with the troughs of the other, much like what was pointed out by Iserles & Nørsett in [11]. This behaviour will be discussed in section 2.5.

The key element in a discussion of the efficiency of this method is the need for moments. Recall that a classical asymptotic method needs no moments, but it breaks down for small ω and the error is not controllable. On the other hand a classical Filon-type method can be made precise also for moderately sized ω , but at the cost of moments. A Filon-type method needs a minimum of 2p moments to obtain asymptotic order p. The combined Filon/asymptotic method is situated between the Filon-type method and the asymptotic method, both in spirit and in terms of requirements. For example, this method can obtain any asymptotic order as well as accuracy for moderately sized ω with the use of only two moments. The asymptotic nature of the method is revealed by the $1/\omega^s$ -factor which indicates that it will perform bad as $\omega \to 0$. For $\omega = 0$ the method does not work, as opposed to the classical Filon-type method which in this case reduces to a classical quadrature method. The combined method can, like the classical Filon-type method, be made precise to a prescribed tolerance by adding more moments. The usefulness is here dictated by the cost of computing moments, as well as the cost of computing $\sigma_m[f]$ and its derivatives. The following example, example 2.3, shows how a combined Filon/asymptotic method performs better than a classical Filon-type method with approximately the same input data. This observation will be elaborated on in section 2.5.1.



Figure 2.2: a) Error for the Filon/asymptotic method with interpolation nodes [-1,0,1](top), and [-1,-1/3,1/3,1](bottom), scaled by ω^3 . b) Error for the classical Filon-type method scaled by ω^3 (same scale as (a))

Example 2.3. Once again we wish to compute with a combined Filon/asymptotic method the integral

$$\int_{-1}^{1} \frac{e^{i\omega x}}{2+x} \mathrm{d}x$$

but this time we include internal nodes. Interpolating $\sigma_1(x) = -1/(2+x)^2$ at the nodes [-1,0,1], and [-1,-1/3,1/3,1] will result in combined schemes requiring three and four moments respectively. That means comparable to the classical Filon-type method from example 2.2, which is obtained by interpolating f(x) = 1/(2+x) with its first derivative at the endpoints requiring four moments. Both this classical method and the above described combined methods have asymptotic order 2. Comparing error plots for the methods(see figure 2.2) we

see that the combined method with nodes [-1, 0, 1] has almost exactly the asymptotic error constant as the classical method when ω increases, whereas the one with nodes [-1, -1/3, 1/3, 1] has a significantly smaller error constant. In figure 2.3 we see how the different methods behaves for small ω . Note that including internal nodes reduces the severity of the singularity. Even for quite small ω the best Filon/asymptotic method is better than the classical method.



Figure 2.3: Log-plot of the error for the Filon/asymptotic method with interpolation nodes [-1, 1](top), [-1, 0, 1](middle) and [-1, -1/3, 1/3, 1](bottom), not scaled. Error for the classical Filon-type method shown as a dotted line

2.3.1 The combined Filon/asymptotic method with stationary points

Extending the method to cater for stationary points is fairly straightforward given Lemma 2.1. Assume in the following that ξ is the only stationary point of order rin [-1, 1]. This requirement is not crucial, it will just simplify otherwise horrific expressions. In the following we will denote by Q_p a method tailored for this problem, like the generalized Filon-type quadrature, which for smooth f bears an error

$$Q_p[f] - I[f] \sim \mathcal{O}(\omega^{-p-1/(r+1)}), \quad \omega \to \infty.$$

Applying the generalized Filon method Q_p^F on the expansion (2.11) yields the

generalized combined Filon/asymptotic method

$$Q_{p,s}^{FA}[f] = \sum_{j=0}^{r-1} \frac{1}{j!} \mu_j(\omega;\xi) \sum_{m=1}^{s} \frac{1}{(-i\omega)^{m-1}} \rho_{m-1}[f]^{(j)}(\xi)$$

$$-\sum_{m=1}^{s} \frac{1}{(-i\omega)^m} \left[\frac{e^{i\omega g(1)}}{g'(1)} \left(\rho_{m-1}[f](1) - \sum_{j=0}^{r-1} \frac{1}{j!} \rho_{m-1}[f]^{(j)}(\xi)(1-\xi)^j \right) - \frac{e^{i\omega g(-1)}}{g'(1)} \left(\rho_{m-1}[f]^{(j)}(\xi)(1-\xi)^j \right) \right]$$

$$(2.15)$$

$$-\frac{1}{g'(-1)} \left(\rho_{m-1}[f](-1) - \sum_{j=0}^{\infty} \frac{1}{j!} \rho_{m-1}[f]^{(j)}(\xi)(-1-\xi)^{j}\right) + \frac{1}{(-i\omega)^{s}} Q_{p}^{F} \left[\rho_{s}[f]\right].$$

 $\rho_m[f]$ are defined as in equation (2.12). Recall that Q_p^F is constructed by interpolating f in the endpoints and ξ (c_1 , c_{ν} and c_q) with multiplicities m_1 , m_{ν} and m_q respectively. Using a generic method Q_p we have the following theorem:

Theorem 2.4. Assume $g'(\xi) = \cdots = g^{(r)}(\xi) = 0$, $g^{(r+1)}(\xi) \neq 0$ and $g'(x) \neq 0$ for $x \in [-1,1] \setminus \{\xi\}$. Let Q_p be a method which for any smooth f has the asymptotic error

$$Q_p[f] - I[f] \sim \mathcal{O}(\omega^{-p-1/(r+1)}), \quad \omega \to \infty.$$

For the combined method $Q_{p,s}$, constructed by applying Q_p on the remainder term in expansion (2.11), applied to any smooth f it is true that

$$Q_{p,s}[f] - I[f] \sim \mathcal{O}(\omega^{-p-s-1/(r+1)}), \quad \omega \to \infty.$$

Proof. Completely analogous to the proof of Theorem 2.3 we get

$$Q_{p,s}[f] - I[f] \sim \frac{1}{(-i\omega)^s} \left(Q_p[\rho_s[f]] - \int_{-1}^1 \rho_s[f](x) e^{i\omega g(x)} \mathrm{d}x \right)$$
$$\sim \frac{1}{(-i\omega)^s} \mathcal{O}(\omega^{-p-1/(r+1)}) = \mathcal{O}(\omega^{-p-s-1/(r+1)}).$$

Again we restrict our treatment to the method $Q_{p,s}^{FA}$ constructed from a generalized Filon-type method.

Example 2.4. The simplest case is a problem with only one stationary point ξ of order one, expanded with one term(as in equation (2.9)). The combined Filon/asymptotic method (2.15) written out is then

$$Q_{p,1}^{FA}[f] = \mu_0(\omega)f(\xi) + \frac{1}{i\omega} \left(\frac{f(1) - f(\xi)}{g'(1)} e^{i\omega g(1)} - \frac{f(-1) - f(\xi)}{g'(-1)} e^{i\omega g(-1)} \right) - \frac{1}{i\omega} Q_p^F \left[\frac{\mathrm{d}}{\mathrm{d}x} \frac{f(x) - f(\xi)}{g'(x)} \right].$$
(2.16)



Figure 2.4: a) The absolute value of the error for the combined Filon/asymptotic method with $\mathbf{c} = [-1, 0, 1]$ (top), together with classical Filon-type method (bottom) in logarithmic scale. b) Combined method with $\mathbf{c} = [-1, -1/2, 0, 1/2, 1]$ (bottom), and the classical Filon-type method(top). All curves are scaled by $\omega^{\frac{5}{2}}$. Logarithmic scale is used in (a) in order to properly represent both curves in the same plot

Example 2.5. The oscillator of the integral

$$\int_{-1}^{1} e^x e^{i\omega \frac{1}{2}x^2} \mathrm{d}x$$

has an order one stationary point at x = 0. Interpolating $\rho_1[f](x) = \frac{d}{dx} \frac{f(x) - f(\xi)}{g'(x)} = \frac{xe^x - e^x + 1}{x^2}$ at the nodes [-1, 0, 1] (using l'Hospital's rule to obtain the value at the stationary point) gives a combined Filon/asymptotic scheme on the form of (2.16).

The predicted error behaviour seems to be confirmed by experiments (see figure 2.4). The proposed scheme needs three moments plus the first generalized moment μ_0 which is constructed from these. A classical Filon-type method requires a total of seven to obtain the same asymptotic order. Figure 2.4 (a) shows that the proposed method has a much higher asymptotic error constant than the classical Filon-type method, however do we only need to add two interpolation nodes, that is two moments, to beat it. See figure 2.4 (b) for illustration.

2.4 Extension to the multivariate case

For the model multivariate highly oscillatory integral we write

$$I[f,\Omega] = \int_{\Omega} f(\mathbf{x}) e^{i\omega g(\mathbf{x})} \mathrm{d}V,$$

where $\Omega \in \mathbb{R}^d$ and $f, g : \Omega \to \mathbb{R}$. Bringing the highly oscillatory quadrature methods into the multivariate setting presents us with a whole set of complications. For example we will have to take into account not only stationary points, \mathbf{x} s.t $\nabla g(\mathbf{x}) = 0$, but also points of resonance, those are boundary points where ∇g is orthogonal to the boundary, i.e. no oscillation along the boundary. For general smooth boundaries resonance will necessarily be a problem, in this case theory is not yet fully developed. Furthermore, computing moments will be even more expensive than in the univariate case. For oscillatory integrals on simplices and polygons we refer to [12] for a theoretical treatment.

In the following we assume that no stationary points or resonance points are present. Furthermore we restrict our treatment to the *d*-dimensional simplex². The Filon-type method is in this case, like in the 1D case, constructed by interpolating in *critical* points, here being the vertices of the simplex. Increasing asymptotic order is done by increasing the number of interpolated derivatives at the vertices.

The point of departure for developing a combined formula will here be the Stokes-type formula for a simplex as presented in [12]:

$$I[f, \mathcal{S}_d] = \frac{1}{i\omega} \int_{\partial \mathcal{S}_d} \mathbf{n}^T(\mathbf{x}) \nabla g(\mathbf{x}) \frac{f(\mathbf{x})}{||\nabla g(\mathbf{x})||^2} e^{i\omega g(\mathbf{x})} \mathrm{d}S$$
$$- \frac{1}{i\omega} \int_{\mathcal{S}_d} \nabla^T \left[\frac{f(\mathbf{x})}{||\nabla g(\mathbf{x})||^2} \nabla g(\mathbf{x}) \right] e^{i\omega g(\mathbf{x})} \mathrm{d}V.$$
(2.17)

Using the formula repeatedly on the remainder term yields an expansion with an integral remainder term. We here state this as a theorem:

²Note that polygons can be tiled by simplices, thus generalising the results for a simplex to the polygon case.

Theorem 2.5. For any smooth f and smooth g without stationary points and subject to the non-resonance condition, it is true that

$$I[f, \mathcal{S}_d] = -\sum_{m=1}^s \frac{1}{(-i\omega)^m} \int_{\partial \mathcal{S}_d} \mathbf{n}^T(\mathbf{x}) \nabla g(\mathbf{x}) \frac{\sigma_{m-1}(\mathbf{x})}{||\nabla g(\mathbf{x})||^2} e^{i\omega g(\mathbf{x})} \mathrm{d}S + \frac{1}{(-i\omega)^s} \int_{\mathcal{S}_d} \sigma_s(\mathbf{x}) e^{i\omega g(\mathbf{x})} \mathrm{d}V, \quad (2.18)$$

where

$$\sigma_0(\mathbf{x}) = f(\mathbf{x})$$

$$\sigma_{m+1}(\mathbf{x}) = \nabla^T \left[\frac{\sigma_m(\mathbf{x})}{||\nabla g(\mathbf{x})||^2} \nabla g(\mathbf{x}) \right].$$

Proof. The proof follows from an iterated use of formula (2.17).

The expansion (2.18) can be carried on to obtain a full expansion for large ω , showing that the value of the integral is asymptotically determined by integrals over the faces of the simplex. Furthermore, by expanding the lower dimensional integrals one repeatedly "pushes" the integrals from faces to edges(lower dimensional faces), a process which terminates at the vertices, indicating that the value of the integral is asymptotically determined by data at the vertices of the simplex. The expansion can also be used to show that the value of the integral $I[f, S_d]$ decays like $\mathcal{O}(\omega^{-d})$.

Now the combined method in all its glorious generality:

Theorem 2.6. Assume Q_p is a quadrature method with asymptotic order p, that is

$$I[f, \mathcal{S}_d] - Q_p[f, \mathcal{S}_d] \sim \mathcal{O}(\omega^{-d-p}), \quad \omega \to \infty.$$

For any smooth f and g, without stationary points and subject to the non-resonance condition, the method

$$Q[f, \mathcal{S}_d] = -\sum_{m=1}^s \frac{1}{(-i\omega)^m} \int_{\partial \mathcal{S}_d} \mathbf{n}^T(\mathbf{x}) \nabla g(\mathbf{x}) \frac{\sigma_{m-1}(\mathbf{x})}{||\nabla g(\mathbf{x})||^2} e^{i\omega g(\mathbf{x})} \mathrm{d}S + \frac{1}{(-i\omega)^s} Q_p[\sigma_s, \mathcal{S}_d]$$
(2.19)

is of asymptotic order s + p.

Proof. As in proof of theorem 2.3, write out the expansion of the error and use the asymptotic error property of Q_p .

This method is not really a quadrature rule per se, as we have not addressed the fact that also the boundary integrals have to be treated somehow. A lower dimensional, thus cheaper, quadrature method might be used. Using the Stokestype formula to reduce the dimension of the boundary integrals until we are left with a formula incorporating data only at the vertices is a possibility, but then also treating the resulting remainder terms with a Filon-type method is preferable in order to retain control over the error.

2.4.1 Quadrature on the 2D simplex

To illustrate the combined Filon/asymptotic approach in the multivariate case we consider the case of the 2D simplex. Assume no stationary points or resonance points are present and write

$$I[f, \mathcal{S}_2] = \int_0^1 \int_0^{1-y} f(x, y) e^{i\omega g(x, y)} \mathrm{d}x \mathrm{d}y.$$

Applying the Stokes-type formula once yields:

$$I[f, \mathcal{S}_{2}] = \frac{1}{i\omega} \int_{0}^{1} \mathbf{n_{1}}^{T} \nabla g(x, 0) \frac{f(x, 0)}{||\nabla g(x, 0)||^{2}} e^{i\omega g(x, 0)} dx \qquad (2.20)$$
$$+ \sqrt{2} \frac{1}{i\omega} \int_{0}^{1} \mathbf{n_{2}}^{T} \nabla g(x, 1-x) \frac{f(x, 1-x)}{||\nabla g(x, 1-x)||^{2}} e^{i\omega g(x, 1-x)} dx$$
$$- \frac{1}{i\omega} \int_{0}^{1} \mathbf{n_{3}}^{T} \nabla g(0, y) \frac{f(0, y)}{||\nabla g(0, y)||^{2}} e^{i\omega g(0, y)} dy$$
$$- \frac{1}{i\omega} \int_{0}^{1} \int_{0}^{1-y} \nabla^{T} \left[\frac{f(x, y)}{||\nabla g(x, y)||^{2}} \nabla g(x, y) \right] e^{i\omega g(x, y)} dx dy$$

with $\mathbf{n_1} = [0, -1], \mathbf{n_2} = \left[\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right]$ and $\mathbf{n_3} = [-1, 0]$ being outer normals as illustrated in figure 2.5.

Example 2.6. Considering the problem

$$I = \int_0^1 \int_0^{1-y} \sin(x+y) e^{i\omega(x-2y)} \mathrm{d}x \mathrm{d}y,$$

we construct a classical Filon-type method of order 2, meaning the error goes down like $\mathcal{O}(\omega^{-4})$, by interpolating function values and derivatives at the vertices. An interpolation point at (1/4, 1/4) is included in order to fix the last parameter in a full third order interpolation polynomial. Thus 10 moments are required. Constructing a combined method with the same asymptotic order from the formula



Figure 2.5



Figure 2.6: (a) The error of the classical Filon-type method, scaled by ω^4 . (b) The combined method, also scaled by ω^4

(2.20), which consists of three univariate and one bivariate integrals, can be done with a first order multivariate method applied to the remainder term and a second order univariate method(error goes like $\mathcal{O}(\omega^{-3})$) on the boundary terms. In total we need four univariate moments per edge plus three bivariate moments for the remainder term. Adding an interpolation point in (1/4, 1/4) for the sake of comparison gives a method with similar accuracy as the classical method, see figure 2.6. We observe that in this case the combined method performs better than the classical method, for general problems the two methods will have comparable accuracy.

Assuming bivariate moments are much harder to compute than univariate moments, the example shows a good improvement of efficiency. On the downside the combined method is harder to implement, and for error control, the error of four quadratures must be balanced, which can pose a problem.

The combined method can also be constructed in a more extreme way, sorting out all information at the vertices as simple terms, and all integrals as remainder terms. Carrying out the computations for the non-resonant 2D simplex problem without stationary points yields the following expression:

$$\begin{split} I &= \frac{1}{(i\omega)^2} \left[\frac{e^{i\omega g(0,0)} f(0,0)}{||\nabla g(0,0)||^2} \left(\frac{g_y(0,0)}{g_x(0,0)} + \frac{g_x(0,0)}{g_y(0,0)} \right) \right. \\ &\quad - \frac{e^{i\omega g(1,0)} f(1,0)}{||\nabla g(1,0)||^2} \left(\frac{g_y(1,0)}{g_x(1,0)} - \frac{g_x(1,0) + g_y(1,0)}{g_x(1,0) - g_y(1,0)} \right) \right. \\ &\quad - \frac{e^{i\omega g(0,1)} f(0,1)}{||\nabla g(0,1)||^2} \left(\frac{g_x(0,1)}{g_y(0,1)} + \frac{g_x(0,1) + g_y(0,1)}{g_x(0,1) - g_y(0,1)} \right) \right] \\ &\quad + \frac{1}{(i\omega)^2} \left[\int_0^1 \frac{\mathrm{d}}{\mathrm{d}x} \left[\frac{f(x,0)g_y(x,0)}{||\nabla g(x,0)||^2g_x(x,0)} \right] e^{i\omega g(x,0)} \mathrm{d}x \right. \\ &\quad - \int_0^1 \frac{\mathrm{d}}{\mathrm{d}x} \left[\frac{f(x,1-x)(g_x(x,1-x) + g_y(x,1-x))}{||\nabla g(x,1-x)||^2(g_x(x,1-x) - g_y(x,1-x)))} \right] e^{i\omega g(x,1-x)} \mathrm{d}x \\ &\quad + \int_0^1 \frac{\mathrm{d}}{\mathrm{d}y} \left[\frac{f(0,y)g_x(0,y)}{||\nabla g(0,y)||^2g_y(0,y)} \right] e^{i\omega g(0,y)} \mathrm{d}y \right] \\ &\quad - \frac{1}{i\omega} \int_0^1 \int_0^{1-y} \nabla^T \left[\frac{f(x,y)}{||\nabla g(x,y)||^2} \nabla g(x,y) \right] e^{i\omega g(x,y)} \mathrm{d}x \mathrm{d}y, \end{split}$$

Note however that this approach will potentially only reduce on the number of univariate moments needed, the bivariate remainder term is still at large. Therefore we will not pursue this approach further.

2.5 Error estimates

In Example 2.2 where the simple univariate case without stationary point was considered, we observed how the troughs in the error plot for a particular Filon/asymptotic method seem to correspond with the peaks of a classical Filon-type method. This is exactly the same observation Iserles and Nørsett made in [10], but then for two different Filon-type methods. The behaviour we have observed can be explained in a similar way. This investigation will also lead to a method for comparing classical Filon-type methods and Filon/asymptotic methods of the same asymptotic order.

Assume in the following that $g'(x) \neq 0$, $-1 \leq x \leq 1$. From the discussion on the asymptotic order of a Filon-type method and equation (2.5) it is clear that

$$Q_p^F[f] - I[f] \sim \frac{e_p^F[f]}{\omega^{p+1}} + \mathcal{O}(\omega^{-p-2}), \quad \omega \to \infty.$$

 $e_p^F[f]/\omega^{p+1}$ is in fact the next term in the expansion of $I[f - \tilde{f}]$, with \tilde{f} being the interpolant of f:

$$e_p^F[f] = \frac{e^{i\omega g(1)}}{(-i)^{p+1}g'(1)} [\sigma_p[\tilde{f}](1) - \sigma_p[f](1)] - \frac{e^{i\omega g(-1)}}{(-i)^{p+1}g'(-1)} [\sigma_p[\tilde{f}](-1) - \sigma_p[f](-1)]$$

By arguing that $\sigma_p[f] = \frac{f^{(p)}}{(g')^p} + a$ linear combination of $f^{(k)}$ multiplied by a function involving derivatives of $g, k = 0, \dots, p-1$, one states that for a Filon-type method the *asymptotic error constant* $|e_p^F|$ can be estimated by

$$\Lambda^F_-[f] \le |e_p^F[f]| \le \Lambda^F_+[f],$$

where

$$\Lambda_{\pm}^{F}[f] = \left| \frac{|\tilde{f}^{(p)}(1) - f^{(p)}(1)|}{|g'(1)|^{p+1}} \pm \frac{|\tilde{f}^{(p)}(-1) - f^{(p)}(-1)|}{|g'(-1)|^{p+1}} \right|.$$

The exact same reasoning can be used to estimate the asymptotic error constant for a combined Filon/asymptotic method $Q_{p,s}^{FA}$. Keeping in mind that the asymptotic order of this method is p + s we can write

$$Q_{p,s}^{FA}[f] - I[f] \sim \frac{e_{p,s}^{FA}[f]}{\omega^{p+s+1}} + \mathcal{O}(\omega^{-p-s-2}), \quad \omega \to \infty$$

Now the Filon-type method is applied to the remainder, so it should be clear that

$$e_{p,s}^{FA}[f] = \frac{e^{i\omega g(1)}}{(-i)^{s+1}g'(1)} [\tilde{\sigma}_s[f]^{(p)}(1) - \sigma_s[f]^{(p)}(1)] - \frac{e^{i\omega g(-1)}}{(-i)^{s+1}g'(-1)} [\tilde{\sigma}_s[f]^{(p)}(-1) - \sigma_s[f]^{(p)}(-1)].$$

Here $\tilde{\sigma}_s[f]$ denotes the interpolant of $\sigma_s[f]$, and $\tilde{\sigma}_s[f]^{(p)}(x)$ its *p*-th derivative evaluated in *x*. This gives

$$\Lambda^{FA}_{-}[f] \le |e^{FA}_{p,s}[f]| \le \Lambda^{FA}_{+}[f],$$

with

$$\Lambda_{\pm}^{FA}[f] = \left| \frac{|\tilde{\sigma}_s[f]^{(p)}(1) - \sigma_s[f]^{(p)}(1)|}{|g'(1)|^{p+1}} \pm \frac{|\tilde{\sigma}_s[f]^{(p)}(-1) - \sigma_s[f]^{(p)}(-1)|}{|g'(-1)|^{p+1}} \right|.$$

Example 2.7. Example 2.2 concerns the problem $\int_{-1}^{1} \frac{e^{i\omega x}}{2+x} dx$, whereby applying a Filon-type method we obtain

$$\tilde{f}(x) = -\frac{1}{9}x^3 + \frac{2}{9}x^2 - \frac{2}{9}x + \frac{4}{9}$$
 and $[\Lambda^F_{-}, \Lambda^F_{+}] = [0.5930, 1.1852].$

The combined Filon/asymptotic method has

$$\tilde{\sigma}_1[f](x) = \frac{4}{9}x - \frac{5}{9}$$
 and $[\Lambda_-^{FA}, \Lambda_+^{FA}] = [1.1852, 1.9259].$

These estimates explain the most significant features of Figure 2.1. For the schemes in Example 2.3 we have for the case $\mathbf{c} = [-1, 0, 1]$:

$$\tilde{\sigma}_1[f](x) = -\frac{11}{36}x^2 + \frac{4}{9}x - \frac{1}{4}, \quad [\Lambda_-^{FA}, \Lambda_+^{FA}] = [0.7037, \ 1.1852],$$

and for $\mathbf{c} = [-1, -\frac{1}{3}, \frac{1}{3}, 1]$:

$$\tilde{\sigma}_1[f](x) = \frac{248}{1225}x^3 - \frac{391}{1225}x^2 + \frac{2668}{11025}x - \frac{2606}{11025}, \quad [\lambda_-^{fa}, \lambda_+^{fa}] = [0.3754, \ 0.6492].$$

these calculations fit well with what has been observed, note in particular how the method with $\mathbf{c} = [-1, 0, 1]$ closely matches the classical filon-type method.

2.5.1 comparing the classical filon and filon/asymptotic methods

now it is time to address the important question: will a combined filon/ asymptotic method get better accuracy than the classical filon-type method from the same information³? for simplicity, consider the fourier case g(x) = x, and also assume derivatives of f are easily available. the maximum error for a filon-type method and a combined filon/asymptotic method, both of asymptotic order p, as ω becomes large are then

$$\lambda_{+}^{f}[f] = |\tilde{f}^{(p)}(1) - f^{(p)}(1)| + |\tilde{f}^{(p)}(-1) - f^{(p)}(-1)|,$$

$$\lambda_{+}^{fa}[f] = |\tilde{\sigma}_{s}[f]^{(p-s)}(1) - \sigma_{s}[f]^{(p-s)}(1)| + |\tilde{\sigma}_{s}[f]^{(p-s)}(-1) - \sigma_{s}[f]^{(p-s)}(-1)|$$

$$= |\tilde{\sigma}_{s}[f]^{(p-s)}(1) - f^{(p)}(1)| + |\tilde{\sigma}_{s}[f]^{(p-s)}(-1) - f^{(p)}(-1)|.$$

now g(x) = x implies that $\sigma_s[f] = f^{(s)}$, and $\tilde{\sigma}_s[f]$ is the interpolant of $f^{(s)}$. we see that both methods have an error which is determined by the interpolant's ability to approximate the *p*th derivative of *f* at the endpoints. the error constant in the filon-type method comes from interpolating *f* and differentiating the interpolant, for the combined approach take *s* derivatives, interpolate, then differentiate. the possibility to more freely chose the placement of the interpolation nodes, not restricted to the endpoints, will also result in a better approximation of the *p*th derivative, explaining at least in part why the combined method performs better than the classical method with the same data. we wish to explore this a bit further.

in the following we will do a small computation to demonstrate what can be gained by using a combined method. consider a method constructed from 2p nodes distributed equidistantly, including endpoints, to approximate the error in a p-1 term asymptotic expansion, that is a $q_{p-1,1}^{fa}$ -type method, compared to a filon-type method of asymptotic order p of minimum complexity q_p^f ? by an order p method of minimum complexity we mean a method constructed by interpolating only p derivatives at the endpoints with no internal nodes, implying that we use the minimum number of moments to attain order p. now bear in mind that equidistant points are by no means optimal, but are just used for the sake of demonstration. these two methods are both are of asymptotic order p and use 2p moments. q_p^f requires p data at each endpoint to interpolate f, it is well known that the error of the hermite interpolation is[5]

$$\tilde{f}(x) - f(x) = \frac{f^{(2p)}(c_1)}{(2p)!}(x+1)^p(x-1)^p,$$

³information here signifies moments.

where $c_1 \in [-1, 1]$. then from rodrigues' formula[1]

$$\tilde{f}^{(p)}(x) - f^{(p)}(x) = \frac{f^{(2p)}(c_1)}{(2p)!} p_p(x) 2^p p!,$$

with $p_p(x)$ being the *p*th legendre polynomial. as $|p_n(\pm 1)| = 1$ we have

$$\lambda_{+}^{f}[f] = 2^{p+1}p! \frac{|f^{(2p)}(c_{1})|}{(2p)!} = |f^{(2p)}(c_{1})| \frac{2^{1-p}\sqrt{\pi}}{\gamma(p+\frac{1}{2})}.$$
 (2.21)

for the $q_{p-1,1}^{fa}$ -type method, we consider the case with n + 1 equidistant nodes, including endpoints. we interpolate $\sigma_{p-1}[f]$, and the interpolation error is now[5]:

$$\tilde{\sigma}_{p-1}[f](x) - f^{(p-1)}(x) = \frac{f^{(p-1+n+1)}(c_2)}{(n+1)!} \prod_{i=0}^n (x-1+i\frac{2}{n}),$$

for $c_2 \in [-1, 1]$. this simplifies to

$$\tilde{\sigma}_{p-1}[f](x) - f^{(p-1)}(x) = \frac{f^{(p+n)}(c_2)}{(n+1)!} \frac{2^{n+1}\gamma(\frac{n}{2}(x+1))}{n^{n+1}\gamma(\frac{n}{2}(x-1))}$$

differentiating gives

$$\tilde{\sigma}_{p-1}[f]'(x) - f^{(p)}(x) = \frac{f^{(p+n)}(c_2)}{(n+1)!} \frac{2^n}{n^n} \frac{\left(\Psi(\frac{n}{2}(x+1)+1) - \Psi(\frac{n}{2}(x-1))\right)\Gamma(\frac{n}{2}(x+1)+1)}{\Gamma(\frac{n}{2}(x-1))},$$

with Ψ being the digamma function. The limit of the above expression as x tends to ± 1 can be found with a bit of effort:

$$\lim_{x \to \pm 1} [\tilde{\sigma}_{p-1}[f]'(x) - f^{(p)}(x)] = f^{(p+n)}(c_2)(\pm 1)^n \frac{2^n}{(n+1)n^n}.$$

Now

$$\Lambda_{+}^{FA}[f] = |f^{(p+n)}(c_2)| \frac{2^{n+1}}{(n+1)n^n}.$$
(2.22)

For the case where the two methods use the same moments n = 2p - 1, and then

$$\Lambda_{+}^{FA}[f] = |f^{(3p-1)}(c_2)| \frac{2^{2p}}{2p \cdot (2p-1)^{2p-1}}.$$

Now we investigate the relative sizes of the two asymptotic error constants.

$$\frac{\Lambda_{+}^{FA}[f]}{\Lambda_{+}^{F}[f]} = \frac{|f^{(3p-1)}(c_{2})|\frac{2^{2p}}{(2p)(2p-1)^{2p-1}}}{|f^{(2p)}(c_{1})|\frac{2^{1-p}\sqrt{\pi}}{\Gamma(p+\frac{1}{2})}} = \frac{|f^{(3p-1)}(c_{2})|}{|f^{(2p)}(c_{1})|}\frac{8^{p}}{4}\frac{\Gamma(p+1/2)}{\sqrt{\pi}p(2p-1)^{2p-1}}$$

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Figure 2.7: Log-plot of the ratio $\frac{8^p}{4} \frac{\Gamma(p+1/2)}{\sqrt{\pi}p(2p-1)^{2p-1}}$

If we use no derivatives, that is p = 1, the ratio is one, and for increasing p the ration is decreasing. In general the derivatives can often be assumed to be of magnitude $|f^{(n)}| \sim L^n$, this will in the limit not alter the conclusion. The significance of the above calculations is most easily appreciated through a plot. Figure 2.7 shows that, assuming the derivatives of f are of the same order of magnitude, the combined Filon/asymptotic method will have a smaller error constant when using the same number of moments.

Example 2.8. As a final little calculation we once again investigate Example 2.3 and the close match between the $\mathbf{c} = [-1, 0, 1]$ combined Filon/asymptotic method and the classical Filon-type method, both of order p = 2. Equation (2.21) with p = 2 gives for the latter

$$\Lambda^F_+[f] \sim \frac{\sqrt{\pi}}{2\frac{3}{4}\sqrt{\pi}} = \frac{2}{3}$$

The c = [-1, 0, 1] combined Filon/asymptotic method has three equidistant nodes, that is n = 2. Equation (2.22) gives,

$$\Lambda_{+}^{FA}[f] \sim \frac{2^3}{3 \cdot 2^2} = \frac{2}{3}$$

This fits well with the close match between the two methods that we observe in example 2.3. Provided that derivatives are of the same order, these methods will in general perform similarly.

We must remark that although the proposed method apparently performs better, it is by no means optimal. The freedom to choose interpolation nodes could be used to minimise the error, placing nodes closer to the boundary would generally be better as derivatives at the boundary would be better approximated, see [10], but this also depends on the size of ω . In the limit $\omega \to \infty$, placing all the nodes at the boundary, increasing the asymptotic order would be best. On the other hand, a more spread out distribution would probably be beneficial for smaller ω . All this seems to make the whole discussion about asymptotic error constants slightly artificial.

2.6 Conclusion

We have demonstrated the feasibility of combining the asymptotic expansion of highly oscillatory integrals and Filon-type methods. Experiments as well as theoretical calculations show that the combined method can achieve better precision than the classical Filon-type method with more or less the same information. The extra cost of the combined method lies mainly in more complicated expressions, especially for cases with several stationary points or in the multivariate case. In order to make a combined method for more general oscillatory integrals we must have an asymptotic expansion with an oscillatory integral remainder. However, such an expansion is not always available.

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Paper II

Asymptotic analysis of numerical steepest descent with path approximations

A. Asheim and D. Huybrechs To appear in Foundations of Computational Mathematics.

Chapter 3

Asymptotic analysis of numerical steepest descent with path approximations

Abstract. We propose a variant of the numerical method of steepest descent for oscillatory integrals by using a low-cost explicit polynomial approximation of the paths of steepest descent. A loss of asymptotic order is observed, but in the most relevant cases the overall asymptotic order remains higher than a truncated asymptotic expansion at similar computational effort. Theoretical results based on number theory underpinning the mechanisms behind this effect are presented.

3.1 Introduction

Consider a highly oscillatory integral of the form

$$I[f] = \int_{-1}^{1} f(x)e^{i\omega g(x)} \,\mathrm{d}x,$$
(3.1)

where ω is a large parameter and f and g are smooth functions called the *amplitude function* and *oscillator* of the integral respectively. Such integrals, often referred to as Fourier-type integrals, appear in a wide area of applications, e.g., highly oscillatory scattering problems in acoustics, electromagnetics or optics [5, 3, 14, 2]. Numerical evaluation of Fourier-type integrals with classical techniques becomes expensive as ω becomes large, which corresponds to a highly oscillatory integral. Typically, a fixed number of evaluation points per wavelength is required to obtain a fixed accuracy, which makes the computational effort at least linear in ω [6].

Asymptotic techniques on the other hand yield approximations that become more accurate as ω increases, making them superior for ω sufficiently large. One of these techniques, the principle of stationary phase [21, 26], states that I[f] asymptotically depends only on f and g in a set of *special points* as $\omega \to \infty$. These points are the endpoints, here x = -1 and x = 1, and stationary points - points where the derivative of g vanishes. At stationary points the integral is locally nonoscillatory. The integral has an asymptotic expansion in inverse powers of ω , with coefficients that depend on the derivatives of f and g at these critical points [16].

A set of particularly effective ways of obtaining the contribution from a special point are the *saddle point methods* [26, 20, 8]. Based on Cauchy's integral theorem, the path of integration can be deformed into the complex plane without changing the value of the integral, provided that f and g are analytic [9]. The *method of steepest descent* is obtained by following a path where g has a constant real part and increasing imaginary part, which renders the integral (3.1) non-oscillatory and exponentially decreasing. This procedure yields separate paths originating from each special point that typically connect at infinity (see Figure 3.1 for an illustration). The result is separate contributions corresponding to each special point. Every one of these contributions is a non-oscillatory integral that can be written as

$$\int_0^\infty \psi(q) e^{-\omega q^r} \mathrm{d}q,\tag{3.2}$$

where ψ is a smooth function, r = 1 for endpoint contributions, and r > 1 for stationary points. These integrals are usually treated with standard asymptotic techniques like Watson's Lemma. The larger class of saddle point methods also contains methods that follow other paths with similar characteristics to the steepest-descent paths, e.g., Perron's method [26].

The asymptotic expansion of I[f] in general diverges, but it can yield very accurate approximations if ω is very large. Still, divergence implies that the error is uncontrollable, which is problematic in the context of numerical computations. Recent research has however produced several numerical methods that



Figure 3.1: The contours of the imaginary part of the oscillator $g(x) = x^2$ in the complex plane and the corresponding paths of steepest descent. Two paths emerge from the endpoints x = -1 and x = 1. They are connected by a path passing through the stationary point at x = 0

exhibit convergence. The Filon-type methods [16, 15, 17] are based on polynomial interpolation of the amplitude f and can deliver errors that are $\mathcal{O}(\omega^{-p})$ for any p, much like truncated asymptotic expansions, but with controllable error for fixed ω . Filon-type methods require that moments $w_k = I[x^k]$ are available, a serious drawback in some cases. Combining asymptotic expansions and Filon-type methods [1] can economise on, but not eliminate the need for moments. Methods that do not rely on moments are the Levin-type methods, due to Levin [19] and extended by Olver [23, 24]. Levin-type methods do not work in the presence of stationary points, but a work-around is provided in [22]. We refer the reader to [11] for a detailed overview of these and other numerical methods.

One of the alternatives is the *numerical method of steepest descent* [12], which is a numerical adaptation of the above described method of steepest descent. Relying on classical numerical integration methods applied to an exact decomposition of the integral, the numerical method of steepest descent has controllable error wherever the exact decomposition is available, and asymptotic error decay $\mathcal{O}(\omega^{-p})$ for any p. The paths of steepest descent can however be difficult to compute, as their computation corresponds to solving a non-linear problem that can in practice only be solved iteratively.

The method of this paper is similar in spirit but based on the practical observation that the exact choice of path is not essential. This observation resonates with the theory behind saddle point methods. A Taylor expansion of the path of steepest descent, which can explicitly be derived from a Taylor expansion of the oscillator function g, is in many cases sufficient. Iterative methods to solve a non-linear problem can therefore be entirely avoided. We obtain a numerical scheme which is relatively simple to implement and cheap to evaluate. The method exhibits high asymptotic order, and the order is in fact higher than one would get from a truncated asymptotic expansion using exactly the same number of derivatives of g. A disadvantage of this approach is that the method again is only asymptotic, even when the decomposition using steepest-descent paths is exact, because the approximate paths may diverge too far away from the exact paths deep into the complex plane – this is the cost of simplicity.

It is the purpose of this paper to analyse the asymptotic order of the proposed explicit numerical saddle-point method. Unlike the numerical adaptation of the steepest-descent method and the other methods for highly oscillatory integrals mentioned above, the asymptotic order does not follow from standard results in asymptotic analysis. A seemingly irregular relation between the number of derivatives of g that are used and the number of quadrature points along the approximate paths of steepest descent can only be explained in terms of elementary number theory. The main result of this paper is formulated and proved in §3.4 in Theorem 3.2.

3.2 The numerical method of steepest descent

In this section we give a brief overview of the numerical method of steepest descent. For a more thorough treatment, see [26] for the classical method of steepest descent, and [12] for particularities on the numerical version. In the following, we will for simplicity assume that all paths may extend to infinity, which implies among other things that f and g should be analytic in a sufficiently large portion of the complex plane. We note that this requirement can be significantly relaxed if so desired [10].

3.2.1 Paths of steepest descent

The method of steepest descent is based on the fact that under the above mentioned restrictions on analyticity, the path of integration can be deformed into the complex plane without changing the value of the integral. A path that follows so-called paths of steepest descent, we shall see, is particularly useful.

For the oscillatory integral (3.1) the path of steepest descent $h_x(p)$ originating at the point x can be found by solving the equation

$$g(h_x(p)) = g(x) + ip.$$
 (3.3)

Subject to the boundary condition $h_x(0) = x$, equation (3.3) is uniquely solvable for small p if $g'(x) \neq 0$. Along the path of steepest descent we have $e^{i\omega g(h_x(p))} =$ $e^{i\omega g(x)}e^{-\omega p}$, which means that the line integral

$$I[f;h_x,P] = e^{i\omega g(x)} \int_0^P f(h_x(p))h'_x(p)e^{-\omega p} \mathrm{d}p,$$

is non-oscillatory and exponentially decreasing. By taking eg. x = -1, the left endpoint of (3.1), this integral is the integration of the integrand $f(x)e^{i\omega g(x)}$ along the path starting at -1.

Along paths of steepest descent originating from different points, $g(h_x(p))$ may have different, constant real parts, hence the paths originating from two different points are in general different and do not connect. Therefore we need to work with at least two paths of steepest descent, one for each endpoint. In addition connecting paths must be introduced. If there are no stationary points, the endpoint paths may connect at infinity by letting $P \to \infty$. In that case, the connecting path has no contribution to the value of the integral. In the presence of stationary points in [-1, 1] however, the connecting path must pass through all of these points and their contributions are not negligible.

Any value $\xi \in [-1,1]$ such that $g'(\xi) = 0$ is called a stationary point. We call ξ a stationary point of order r-1 if $g^{(i)}(\xi) = 0$ for i = 1, 2, ..., r-1, and $g^{(r)}(\xi) \neq 0.^1$. The canonical example of a stationary point of order r-1 at x = 0 is $g(x) = x^r$. At a stationary point, equation (3.3) may have several solutions. In particular, if ξ is a stationary point of order r-1 > 0, then there are r different paths, $h_{\xi,j}$, j = 1, ..., r, emerging from ξ . Since the connecting path passes trough ξ only once, exactly two of these paths are relevant. We denote these two paths by h_{ξ,j_1} and h_{ξ,j_2} . Each of these paths corresponds to an integral of the form

$$I[f; h_{\xi,j}, P] = e^{i\omega g(\xi)} \int_0^P f(h_{\xi,j}(p)) h'_{\xi,j}(p) e^{-\omega p} \, \mathrm{d}p.$$

Again, letting $P \to \infty$ eliminates contributions from paths connecting h_{ξ} with other steepest-descent paths, under above mentioned assumptions. Writing

$$I[f;h_x] = \lim_{P \to \infty} I[f;h_x,P],$$

the integral (3.1) is represented as a sum of contributions

$$I[f] = I[f; h_{-1}] - I[f; h_{\xi_1, j_1}] + I[f; h_{\xi_1, j_2}] + \dots - I[f; h_{\xi_n, j_1}] + I[f; h_{\xi_n, j_2}] - I[f; h_1],$$

where ξ_1, \ldots, ξ_n are stationary points. We will in the rest of this paper concentrate on integrals of the type I[f; h], hereafter referred to as steepest-descent integrals.

¹Note that with this definition any point which is not a stationary point, these may well include endpoints, may be considered points of order 0

3.2.2 Numerical evaluation of steepest-descent integrals

Steepest-descent integrals can be approximated efficiently with Gaussian quadrature. This is the observation behind the numerical method of steepest descent, which we shall briefly explain here.

For convenience, we introduce the notation

$$f_x(p) = f(h_x(p))h'_x(p).$$

The contribution from an endpoint becomes

$$I[f;h_x] = e^{i\omega g(x)} \int_0^\infty f_x(p) e^{-\omega p} dp = \frac{e^{i\omega g(x)}}{\omega} \int_0^\infty f_x(\frac{t}{\omega}) e^{-t} dt.$$
(3.4)

Since $f_x(t/\omega)$ is smooth, this integral can be computed efficiently with classical Gauss-Laguerre quadrature for the weight function e^{-t} [6]. Applying an *n*-point quadrature yields an approximation with error $\mathcal{O}(\omega^{-2n-1})$ [12]. Truncating the asymptotic expansion after *n* terms yields only $\mathcal{O}(\omega^{-n-1})$ asymptotic error, but requires the same number of evaluations of f.

For the contribution from a stationary point things are a little different. When ξ is a stationary point of order r - 1 > 0, $h_{\xi}(p)$ behaves as $p^{1/r}$ near p = 0 and $h'_{\xi}(p)$ has a $p^{-(r-1)/r}$ singularity [9]. This singularity can be canceled by the substitution $p = q^r$. The contribution is now written

$$I[f;h_{\xi}] = r e^{i\omega g(\xi)} \int_{0}^{\infty} f_{\xi}(q^{r}) q^{r-1} e^{-\omega q^{r}} dq \qquad (3.5)$$
$$= \frac{r e^{i\omega g(\xi)}}{\omega} \int_{0}^{\infty} f_{\xi}(\frac{t^{r}}{\omega}) t^{r-1} e^{-t^{r}} dt.$$

This is an integral of the form (3.2). Since $f_{\xi}(\frac{t^r}{\omega})t^{r-1}$ is a smooth function, the integral can be efficiently approximated by Gaussian quadrature with weight function e^{-t^r} . We note that it may be beneficial to merge the two contributions from a stationary point into a single integral over the whole real line. For example, in the case of a first order stationary point (r = 2), classical Gauss-Hermite quadrature can be applied [7]. In this exposition, however, we will only work with integrals on the half-space.

The result of applying an *n*-point Gaussian quadrature leads to an approximation with an error which is $\mathcal{O}(\omega^{-(2n+1)/r})$ as $\omega \to \infty$ [7, Lemma 1]. In contrast, truncating the asymptotic expansion after *n* terms yields only $\mathcal{O}(\omega^{-(n+1)/r})$ asymptotic error, but requires the same number of evaluations of *f*.

3.3 A numerical saddle point method

Finding the path of steepest descent means solving equation (3.3). This is a nonlinear equation and solving it amounts to computing the inverse function g^{-1} , which in practical applications may be difficult to achieve. The rationale in this section is that in many cases it is sufficient to have only a rough approximation of the exact steepest-descent path. If not, then the rough approximation is still useful as a starting value for, e.g., Newton iterations to solve the non-linear equation numerically.

Here, we obtain a local approximation of the path by means of its Taylor series around x. Only derivatives of g at x are used to construct this approximation. This approximate path may diverge away from the actual steepest-descent path deep into the complex plane. However, this is not a problem in practice provided ω is large: because the quadrature points cluster towards x as ω grows, as can be seen from equations (3.4) and (3.5), a good approximation close to the real axis is generally sufficient.

3.3.1 Local paths at endpoints

In the case of the steepest-descent path emerging from an endpoint, we assume that the path is of the form

$$h_x(p) = x + \sum_{j=1}^{\infty} a_j p^j.$$
 (3.6)

Note that we already incorporated the boundary condition $h_x(0) = x$. Substitution into equation (3.3) gives

$$g\left(x + \sum_{j=1}^{\infty} a_j p^j\right) = g(x) + ip.$$

Taking the Taylor expansion of g around x yields the equation

$$\sum_{k=1}^{\infty} \frac{(\sum_{j=1}^{\infty} a_j p^j)^k}{k!} g^{(k)}(x) = ip.$$
(3.7)

The coefficients can now be obtained by series inversion. The first few coefficients are given explicitly by, with evaluation in x implied,

$$a_{1} = \frac{i}{g'}, \qquad a_{2} = \frac{1}{2} \frac{g''}{(g')^{3}},$$

$$a_{3} = \frac{i}{6(g')^{5}} \left(g'g''' - 3(g'')^{2}\right), \qquad (3.8)$$

$$a_{4} = -\frac{1}{24} \frac{1}{(g')^{7}} \left(g^{(4)}(g')^{2} - 10g'g''g''' + 15(g'')^{3}\right).$$

In general, a_k is given in terms of derivatives of g up to order k.

We define the local path h_x by truncating the series of h_x after m terms,

$$\tilde{h}_x(p) = x + \sum_{j=1}^{m-1} a_j p^j.$$
(3.9)

This means that the left and right hand side of (3.3) match up to order m,

$$g(\tilde{h}_x(p)) = g(x) + ip + \mathcal{O}(p^m), \qquad p \to 0.$$
(3.10)

From this path we can define the steepest-descent integral with an approximated path, using the notation $\tilde{f}_x(p) = f(\tilde{h}_x(p))\tilde{h}'_x(p)$ and $\tilde{g}_x(p) = g(\tilde{h}_x(p))$,

$$I[f; \tilde{h}_x, P] = \int_0^P \tilde{f}_x(p) e^{i\omega \tilde{g}_x(p)} \mathrm{d}p.$$
(3.11)

We shall later evaluate this integral numerically. The numerical approximation will serve as an approximation to the infinite integral $I[f; h_x]$, we shall see that this is indeed justified in §3.4.1.

3.3.2 Local paths at stationary points

We now turn our attention to paths passing through stationary points. Let x be a stationary point of order r - 1, meaning that $g'(x) = \ldots = g^{(r-1)}(x) = 0$, but $g^{(r)}(x) \neq 0$. Expanding the path starting at x in integer powers of p is not possible, since $h_x(p)$ is singular at p = 0. This can also be seen from equation (3.7): the first r - 1 terms in the expansion of g in the left hand side would be zero, which makes it impossible to match the right hand side of the equation. However, proceeding as in §3.2.2, the substitution $p = q^r$ eliminates this problem. Thus, we assume a path of the form

$$h_x(p) = x + \sum_{j=1}^{\infty} a_j p^{j/r}.$$
 (3.12)

Note that the function $h_x(q^r)$ is analytic in q. Plugging this ansatz into equation (3.3) for the path of steepest descent yields

$$\sum_{k=r}^{\infty} \frac{(\sum_{j=1}^{\infty} a_j p^{j/r})^k}{k!} g^{(k)}(x) = ip.$$
(3.13)

The first coefficient is easily obtained,

$$a_1 = \sqrt[r]{\frac{ir!}{g^{(r)}(x)}}.$$
(3.14)

The r-th root in this expression has r branches in the complex plane, corresponding to the r different paths near the stationary point. More coefficients can be computed recursively. In the case of an order one stationary point, the first four coefficients are, with evaluation in x implied,

$$a_{1} = \pm \sqrt{\frac{2i}{g''}}, \qquad a_{2} = -\frac{i}{3} \frac{g^{(3)}}{(g'')^{2}},$$

$$a_{3} = \pm \sqrt{\frac{2i}{g''}} \frac{i}{36(g'')^{3}} \left(5(g''')^{2} - 3g''g^{(4)} \right), \qquad (3.15)$$

$$a_{4} = \frac{1}{270} \frac{1}{(g'')^{5}} \left(40(g''')^{3} - 45g^{(4)}g'''g'' + 9g^{(5)}(g'')^{2} \right).$$

Explicit expressions for the coefficients can be found for general r. We refer the reader to [25] for a general description of such explicit expressions.

As in the endpoint case, we form an approximated path by truncating (3.12) after m terms,

$$\tilde{h}_x(p) = x + \sum_{j=1}^{m-1} a_j p^{j/r}.$$
(3.16)

This means that the both sides of (3.3) match up to order $\frac{r+m-1}{r}$,

$$g(\tilde{h}_x(p)) = g(x) + ip + \mathcal{O}(p^{\frac{r+m-1}{r}}), \qquad p \to 0.$$
 (3.17)

This expression agrees with (3.10) for r = 1. Next, we form the integral

$$I[f; \tilde{h}_x, P] = \int_0^P \tilde{f}_x(p) e^{i\omega \tilde{g}_x(p)} dp.$$

=
$$\int_0^Q r q^{r-1} \tilde{f}_x(q^r) e^{i\omega \tilde{g}_x(q^r)} dq.$$
 (3.18)

with $Q = P^{1/r}$.

3.3.3 Numerical evaluation

As noted in section §3.2.2, it is advantageous to evaluate the half-space integral $I[f, h_x]$ with Gaussian quadrature. Though the integral $I[f, \tilde{h}_x, P]$ is finite, we intend to apply Gaussian half-space quadrature here as well.

For the numerical evaluation of steepest-descent integrals with approximated paths, we rewrite (3.18) as

$$I[f; \tilde{h}_x, P] = \int_0^Q r q^{r-1} \tilde{f}_x(q^r) e^{i\omega \tilde{g}_x(q^r) + \omega q^r} e^{-\omega q^r} \mathrm{d}q.$$
(3.19)

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Note that (3.11) is a special case of (3.19) with r = 1, so that we can treat the cases of endpoints and stationary points simultaneously. A change of variables $q = \omega^{-1/r} t$ gives the form

$$I[f; \tilde{h}_x, P] = \frac{r}{\omega} \int_0^{Q\omega^{1/r}} t^{r-1} \tilde{f}_x(t^r/\omega) e^{i\omega \tilde{g}_x(t^r/\omega) + t^r} e^{-t^r} \mathrm{d}t.$$

This integral can be evaluated with the same Gaussian half-space quadrature rules with weight function e^{-t^r} that were used on the exact steepest-descent integrals. To be precise, if that quadrature rule is given by points x_i and weights w_i , then we propose the approximation

$$I[f;\tilde{h}_x,P] \approx Q[f;\tilde{h}_x] := \frac{r}{\omega} \sum_{i=1}^n w_i x_i^{r-1} \tilde{f}_x \left(\frac{x_i^r}{\omega}\right) e^{i\omega \tilde{g}_x \left(\frac{x_i^r}{\omega}\right) + x_i^r}.$$
 (3.20)

We expect that this quadrature rule provides a good approximation to $I[f; h_x, P]$. This is what we examine next in §3.4.

3.4 Asymptotic error analysis

Thus far, we have presented a way of obtaining a numerical approximation of $I[f; \tilde{h}_x, P]$. We will show first in §3.4.1 that this finite saddle-point integral is a good (asymptotic) approximation to the infinite steepest-descent integral $I[f; h_x]$. Next, we shall investigate in §3.4.2 the numerical approximation of $I[f; \tilde{h}_x, P]$ by Gaussian quadrature. Theorem 3.2 gives the asymptotic order of this approximation. Its proof follows in §3.4.3 and §3.4.4.

3.4.1 The error of using truncated approximate paths

In the method outlined in section §3.3, we replaced the exact path of steepest descent h_x originating at x with an approximation \tilde{h}_x that is valid only near x. By our assumptions of analyticity, the path taken does not change the value of the integral. However, since the approximate path may diverge away from the exact path for large P, the limit $P \to \infty$ may result in both paths leading into different sectors of the complex plane. It is clear that the integral along the approximate path should be truncated at finite P to avoid this. In the following theorem and corollary, we prove that the difference between the exact steepest-descent integral $I[f; h_x]$ and the truncated integral $I[f; \tilde{h}_x, P]$ is exponentially small as $\omega \to \infty$, provided P is sufficiently small. This implies that using a numerical approximation of $I[f; \tilde{h}_x, P]$ is justified.



Figure 3.2: Illustration of the exact (continuous) and approximate (dashed) steepestdescent paths. The curve Γ connects a truncation of these two paths

Theorem 3.1. Let $x \in [-1, 1]$ be a point of order r - 1. Assume f and g are analytic, and let $\tilde{h}_x(p)$ be an *m*-term approximation to the exact path $h_x(p)$ as in (3.16) with m > 1. Then a constant $P_0 > 0$ exists, such that

$$I[f; h_x, P] - I[f; h_x, P] = \mathcal{O}(\omega^{-n}), \quad \forall n > 0, \quad \forall P < P_0.$$

Proof. By Cauchy's integral theorem we have

$$I[f; \tilde{h}_x, P] - I[f; h_x, P] = \int_{\Gamma} f(s) e^{i\omega g(s)} \mathrm{d}s,$$

where Γ is any simple path connecting $h_x(P)$ and $\tilde{h}_x(P)$. In the following, we choose Γ to be the straight line. We intend to show that the integrand is exponentially small along all of Γ .

Let us expand g in a Taylor series around $h_x(P)$. We have $g(x + \delta) = g(x) + O(\delta^r)$ and $g^{(j)}(x + \delta) = O(\delta^{r-j})$. Since $h_x(p) = O(p^{1/r})$, we find that

$$g^{(j)}(h_x(p)) = \mathcal{O}(p^{(r-j)/r}).$$
 (3.21)

We have by construction that $h_x(p) - \tilde{h}_x(p) = \mathcal{O}(p^{m/r})$ and therefore,

$$\gamma - h_x(P) = \mathcal{O}(P^{m/r}), \qquad \gamma \in \Gamma, \quad P \to 0.$$
 (3.22)

To conclude, we note that for sufficiently small P, such that Γ lies in the radius of convergence of the Taylor series of g at $h_x(P)$, and for any $\gamma \in \Gamma$, we may write

$$g(\gamma) = g(h_x(P) + \gamma - h_x(P)) = \sum_{j=0}^{\infty} g^{(j)}(h_x(P)) (\gamma - h_x(P))^j$$

= $g(x) + iP + \sum_{j=1}^{\infty} g^{(j)}(h_x(P)) (\gamma - h_x(P))^j.$

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Now, if m > 1, by considering (3.22) and (3.21), the term iP dominates the terms in the summation as $P \to 0$. Therefore g has positive imaginary part along Γ , again for sufficiently small P. It follows in that case that the integrand is exponentially small along all of Γ .

Corollary 3.1. Under the assumptions of Theorem 3.1, provided $P < P_0$,

$$I[f;h_x] - I[f;h_x,P] = \mathcal{O}(\omega^{-n}), \quad \forall n > 0, \quad \omega \to \infty.$$

Proof. We have

$$I[f;h_x] = I[f;h_x,P] + \int_P^\infty \psi(q) e^{-\omega q^r} \mathrm{d}q,$$

where $\psi(q)$ is analytic in q. It follows from repeated integration by parts that

$$I[f;h_x] - I[f;h_x,P] = \mathcal{O}(\omega^{-n}), \qquad \forall n > 0 \qquad \omega \to \infty.$$

The result follows from this and Theorem 3.1.

3.4.2 Asymptotic error of the numerical approximation

Since replacing the paths does not lead to a loss in asymptotic order, the order of the overall method relies on the order of the numerical approximation of $I[f; \tilde{h}_x, P]$. We evaluate the latter by a quadrature rule. A quadrature rule with n points and with order d with respect to the weight function e^{-x^r} satisfies the conditions

$$\int_0^\infty x^j e^{-x^r} \, \mathrm{d}x = \sum_{k=1}^n w_k \, x_k^j, \quad j = 0, \dots, d-1.$$
(3.23)

Using such a rule for the steepest-descent integral leads to an asymptotic error of size $\mathcal{O}(\omega^{-(d+1)/r})$ [7, Th.2]. When using an approximate path, we have the following result. Note that by integer division $d \setminus \beta$, we mean that the real quantity d/β is rounded towards the nearest smaller integer.

Theorem 3.2. Assume x is either a regular point, r = 1, or a stationary point of order r - 1 > 0. An approximation $I[f; \tilde{h}_x, P]$ to the steepest-descent integral $I[f; h_x]$ is constructed by replacing the path h_x with its m-term Taylor expansion \tilde{h}_x , with m > 1 and with $P < P_0$ sufficiently small as in Theorem 3.1. Let $Q[f; \tilde{h}_x]$, given by (3.20), denote the approximation to $I[f; \tilde{h}_x, P]$, obtained through an n-point quadrature rule of order d that satisfies the conditions (3.23).

Define $\beta = r + m - 1$, $k = d \setminus \beta$ and $l = d \mod \beta$. Then

$$I[f;h_x] - Q[f;\tilde{h}_x] = \begin{cases} \mathcal{O}(\omega^{-\frac{d+1}{r}+k}), & \text{if } l \le m-1, \\ \mathcal{O}(\omega^{-\frac{d+1}{r}+k+\frac{l-(m-1)}{r}}), & \text{if } l > m-1, \end{cases}$$
(3.24)

 \square
for $\omega \to \infty$. In particular, for r = 1 we have

$$I[f;h_x] - Q[f;\tilde{h}_x] = \mathcal{O}(\omega^{-d-1+d\backslash m}).$$

We can also formulate an upper bound for the exponents in (3.24) that avoids integer arithmetic.

Corollary 3.2. Under the same conditions as in Theorem 3.2, we have

$$I[f;h_x] - Q[f;\tilde{h}_x] = \mathcal{O}(\omega^{-\frac{d+1}{r} + \frac{d}{\beta}}).$$
(3.25)

Proof. For the first case of (3.24), note that $k = d \setminus \beta \le d/\beta$. For the second case, assume that l = K + m - 1 with 0 < K < r. Then $k + \frac{l - (m - 1)}{r} = k + \frac{K}{r} < k + \frac{K + m - 1}{r + m - 1} = \frac{d}{\beta}$.

Let us first compare the result of Theorem 3.2 to the result based on using the exact path. One incurs a loss of minimum $k = d \setminus \beta = d \setminus (r + m - 1)$. In order to achieve the full order (d + 1)/r, one should at least have k = 0, meaning $d < \beta$,

$$m > d - r + 1.$$

Full order is then achieved if $l \le m-1$, which is always true whenever r = 1, and more likely to be violated for larger r. In the converse case, we have a maximum order loss of one.

Next, we compare to the result based on using a truncated asymptotic expansion. This is more involved. An s-term expansion has asymptotic error $\mathcal{O}(\omega^{-(s+1)/r})$ and requires the values $g^{(j)}(x)$, $j = 0, \ldots, r + s - 1$ [16]. Using these same values, we can afford m = s + 1. The asymptotic expansion also requires the s values $f^{(j)}(x)$, $j = 0, \ldots, s - 1$, whereas the proposed method needs n evaluations of f and g. We choose n = s for the comparison and continue by counting evaluations of f or any of its derivatives. For the asymptotic expansion, s values of f lead to order $\frac{s+1}{r}$. A Gaussian quadrature rule with respect to the weight function e^{-x^r} yields d = 2s. By Corollary 3.2, the proposed numerical saddle-point method then yields an order greater than or equal to

$$\frac{d+1}{r} - \frac{d}{\beta} = \frac{2s+1}{r} - \frac{2s}{r+s} = \frac{s+1}{r} + \frac{s}{r} \left[\frac{s-r}{r+s} \right]$$

Thus we are guaranteed to do at least as good as the asymptotic expansion whenever $s \ge r$.

Note that in the above, we ignored the evaluations of g in the complex plane. This is justified in a setting where many integrals of the form I[f] need to be evaluated for the same oscillator g, for example when computing moments for later use in Filon-type quadrature [16].

Both these calculations show that the proposed method compares well to both the method with exact paths and asymptotic expansions when r is relatively small. In real-life applications we do however not expect to encounter cases with r being large, we will typically have r = 1 or r = 2.

3.4.3 Supporting lemmas for the proof of Theorem 3.2

We once again rewrite the integral $I[f; \tilde{h}_x, P]$ in the following form:

$$I[f, \tilde{h}_x, P] = e^{i\omega g(x)} \int_0^Q \tilde{\psi}(q) e^{i\omega R_{r+m-1}(q)} e^{-\omega q^r} \mathrm{d}q, \qquad (3.26)$$

where r-1 is the order of the point x, $R_{\beta}(q)$ is a function of the form

$$R_{\beta}(q) = q^{\beta} \sum_{j=0}^{\infty} r_j q^j.$$
(3.27)

To be precise, one sees by comparing to (3.19) that this means

$$R_{r+m-1}(q) = \tilde{g}_x(q^r) - iq^r - g(x),$$

and

$$\tilde{\psi}(q) = r \,\tilde{f}_x(q^r) \, q^{r-1}.$$

It is important in the following that the function $R_{r+m-1}(q)$ indeed vanishes to order r + m - 1, which can be seen by inserting (3.17) into (3.19), and that the function $\tilde{\psi}(q)$ is a smooth function independent of ω .

The following lemma is a generalization of Lemma 2.1 in [7]. That lemma characterized the asymptotic order of a scaled quadrature rule applied to a steepest-descent integral of the form (3.2). Assume an *n*-point quadrature rule is given that satisfies the conditions (3.23). It was proved in [7] that, for a function u(x) analytic in x = 0, the quadrature approximation behaves as

$$\int_0^\infty u(x)e^{-\omega x^r} \, \mathrm{d}x - \omega^{-1/r} \sum_{k=1}^n w_k u(x_k \omega^{-1/r}) = \mathcal{O}(\omega^{-(d+1)/r}).$$

Here, we will allow the integrand to depend on ω in a benign manner and show that the asymptotic order changes in a way that reflects the possible growth or decay of the integrand as a function of ω .

Lemma 3.1. Assume an *n*-point quadrature rule is given such that conditions (3.23) hold. Let $u(x; \omega)$ be analytic in x = 0 with a positive radius of convergence R for each $\omega \ge \omega_0$,

$$u(x;\omega) = \sum_{j=0}^{\infty} a_j(\omega) x^j, \quad |x| < R,$$
(3.28)

and such that $a_j = \mathcal{O}(\omega^{\gamma_j})$ with $\gamma_j \in \mathbb{R}$. If 0 < P < R, then

$$\int_0^P u(x;\omega)e^{-\omega x^r} \,\mathrm{d}x - \omega^{-1/r} \sum_{k=1}^n w_k u(x_k \omega^{-1/r};\omega) = \mathcal{O}(\omega^{\max_{j\geq d} \gamma_j - \frac{j+1}{r}}).$$

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Proof. We have

$$\int_0^P u(x;\omega)e^{-\omega x^r} \,\mathrm{d}x = \sum_{j=0}^\infty a_j(\omega) \int_0^P x^j e^{-\omega x^r} \,\mathrm{d}x$$

Using integration by parts, as in the proof of Corollary 3.1, we find that

$$\int_0^\infty x^j e^{-\omega x^r} \, \mathrm{d}x - \int_0^P x^j e^{-\omega x^r} \, \mathrm{d}x = \mathcal{O}(\omega^{-m}), \qquad \forall m \in \mathbb{N}$$

Next, it is straightforward to verify that

$$\int_0^\infty x^j e^{-\omega x^r} \, \mathrm{d}x - \omega^{-1/r} \sum_{k=1}^n w_k \, (x_k \omega^{-1/r})^j = \begin{cases} 0, & j < d, \\ \mathcal{O}(\omega^{-(j+1)/r}), & j \ge d. \end{cases}$$

The first case follows from exactness of the quadrature rule for polynomials up to degree d-1. The second case follows because both terms in the left hand side have the given size: the integral can be computed explicitly, the summation contains the factor $\omega^{-(j+1)/r}$.

Combining all of the above proves the result. Note that $u(x; \omega)$ is evaluated in the points $x_k \omega^{-1/r}$ which, for sufficiently large ω , lie in the radius of convergence of u.

Finally, we will examine the asymptotic size of functions of the form $e^{\omega \eta(x)}$ and their derivatives. In order to obtain the result, we use a version of Faà di Bruno's formula expressed with integer partitions. A partition of an natural number $n \ge 0$ is a way of writing it as a sum of natural numbers. The number of different ways to do this is the partition number of n, denoted a(n). We write a partition pof the integer n as an array $p = (p_1, p_2, \ldots, p_n)$, where p_j is the number of times the integer j occurs in the sum, i.e.,

$$\sum_{j=1}^{n} j \, p_j = n. \tag{3.29}$$

See, e.g., [4] for a detailed treatment of partitions and [18] for Faà di Bruno's formula, which we recall in the following Lemma.

Lemma 3.2 (Faà di Bruno's Formula). If g and f are functions that are sufficiently differentiable, then

$$\frac{\mathrm{d}^n}{\mathrm{d}x^n}g(f(x)) = \sum \frac{n!}{p_1!p_2!\dots p_n!}g^{(k)}(f(x))\Big(\frac{f'(x)}{1!}\Big)^{p_1}\Big(\frac{f''(x)}{2!}\Big)^{p_2}\dots\Big(\frac{f^{(n)}(x)}{n!}\Big)^{p_n},$$

where the sum is over all partitions p of n with entries p_1, p_2, \ldots, p_m , and $k = p_1 + p_2 + \ldots + p_n$.

Lemma 3.3. Let $R_{\beta}(q)$ be defined by (3.27) for an integer $\beta > 0$. The derivatives of $e^{\omega R_{\beta}(q)}$, evaluated at q = 0, have an expansion of the form

$$\frac{\mathrm{d}^n}{\mathrm{d}q^n} e^{\omega R_\beta(q)}\Big|_{q=0} = \sum_{j=0}^{n\setminus\beta} b_j \,\omega^j, \qquad \omega \to \infty,$$

where \setminus denotes integer division.

Proof. It is clear that

$$R_{\beta}^{(j)}(0) = 0, \qquad 0 \le j < \beta.$$
 (3.30)

Using Faà di Bruno's Formula (Lemma 3.2), we have

1.

$$\begin{aligned} \frac{\mathrm{d}^{n}}{\mathrm{d}q^{n}} e^{\omega R_{\beta}(q)} \Big|_{q=0} &= \\ e^{\omega R_{\beta}(0)} \sum \frac{n!}{p_{1}! p_{2}! \dots p_{n}!} \Big(\frac{\omega R_{\beta}'(q)}{1!}\Big)^{p_{1}} \Big(\frac{\omega R_{\beta}''(q)}{2!}\Big)^{p_{2}} \dots \Big(\frac{\omega R_{\beta}^{(n)}(q)}{n!}\Big)^{p_{n}} \\ &= \sum \frac{n!}{p_{1}! p_{2}! \dots p_{n}!} \Big(\frac{\omega R_{\beta}^{(\beta)}(q)}{\beta!}\Big)^{p_{\beta}} \Big(\frac{\omega R_{\beta}^{(\beta+1)}(q)}{(\beta+1)!}\Big)^{p_{\beta+1}} \dots \Big(\frac{\omega R_{\beta}^{(n)}(q)}{n!}\Big)^{p_{n}}, \end{aligned}$$

where the sum is over all partitions p of n. The last line follows from equation (3.30). Clearly, each of the terms in this sum is proportional to $\omega^{\sum_{j=\beta}^{n} p_j}$. It is also clear that the expansion consists of positive integer powers of ω . To find the dominating term, we maximise the expression $\sum_{j=\beta}^{n} p_j$ over the set of all partitions of n. It remains only to prove that

$$\sum_{j=\beta}^{n} p_j \le n \backslash \beta, \quad \forall \, p \text{ partitions of } n.$$

Assume a partition q of n exists such that

$$\sum_{j=\beta}^{n} q_j = n \backslash \beta + M,$$

with M > 0. From q we can construct another partition \tilde{q} as follows. We let $\tilde{q}_{\beta} = n \setminus \beta + M$ and $\tilde{q}_j = 0, j > \beta$. It follows from our construction that

$$\sum_{j=\beta}^{n} j q_j \ge \sum_{j=\beta}^{n} j \tilde{q}_j = \beta(n \backslash \beta + M) > n.$$

No matter how we choose \tilde{q}_j for $j < \beta$, \tilde{q} can never satisfy the summation property (3.29) and neither can q. This proves the result *reductio ad absurdum*.

The final lemma concerns the maximal exponent of ω that may arise in the result of Lemma 3.1.

Lemma 3.4. Assume that r and β are integers such that $\beta > r$ and define the sequence

$$s_j = j \backslash \beta - \frac{j}{r}.$$

For any positive integer d, let $k = d \setminus \beta$ and $l = d \mod \beta$. The maximum of $\{s_j\}_{j=d}^{\infty}$ is

$$\max_{j \ge d} s_j = \begin{cases} k - \frac{d}{r}, & \text{if } l \le \beta - r, \\ k + 1 - \frac{(k+1)\beta}{r}, & \text{if } l > \beta - r. \end{cases}$$

Proof. For the integer division we have the identity

$$j \setminus \beta = \frac{j}{\beta} - \frac{1}{\beta} (j \mod \beta).$$
 (3.31)

This means that

$$s_j = j(\frac{1}{\beta} - \frac{1}{r}) - \frac{1}{\beta}(j \mod \beta).$$

The first of these terms is decreasing monotonically. The second term is nonincreasing, except when the integer part of j/β changes. This implies that the largest element in the sequence for $j \ge d$ is either the first element, s_d , or $s_{n\beta}$ for some integer n. In the latter case, we have

$$s_{n\beta} = n(1 - \beta/r),$$

which again is decreasing. This means that a maximum must occur at the smallest admissible n. This is n = k, when d is a multiple of β , and n = k + 1 otherwise. This leads to $s_{k\beta} = s_d$ as above or $s_{(k+1)\beta}$.

From the identity (3.31), we find that the corresponding element is either

$$s_d = d \backslash \beta - \frac{d}{r} = k - \frac{d}{r}$$

or

$$s_{(k+1)\beta} = (k+1)\beta\backslash\beta - \frac{(k+1)\beta}{r} = k+1 - \frac{(k+1)\beta}{r}$$

One easily verifies that the former is larger than the latter if $l < \beta - r$. They are equal if $l = \beta - r$.

3.4.4 Proof of Theorem 3.2

We assembled enough results in §3.4.3 to state a short proof of Theorem 3.2. In the following, let $\beta = r + m - 1$.

Proof. Leibniz' formula gives the derivatives of the integrand of (3.26) as the sum

$$\frac{\mathrm{d}^n}{\mathrm{d}q^n} \left[\tilde{\psi}(q) e^{i\omega R_\beta(q)} \right] = \sum_{j=0}^n \binom{n}{j} \left[\frac{\mathrm{d}^j}{\mathrm{d}q^j} e^{i\omega R_\beta(q)} \frac{\mathrm{d}^{n-j}}{\mathrm{d}q^{n-j}} \tilde{\psi}(q) \right].$$

Lemma 3.3 applied to each of the these terms gives an expansion of the form,

$$\frac{\mathrm{d}^n}{\mathrm{d}q^n} \left[\tilde{\psi}(q) e^{i\omega R_\beta(q)} \right]_{q=0} = \sum_{j=0}^{n \setminus \beta} c_j \, \omega^j.$$

Hence, a Taylor series around q = 0 has coefficients that are $\mathcal{O}(\omega^{n\setminus\beta})$.

All conditions of Lemma 3.1 are satisfied and we can conclude that the error of the quadrature approximation is

$$I[f; \tilde{h}_x, P] - Q[f; \tilde{h}_x] = \mathcal{O}(\omega^{\max_{j \ge d} j \setminus \beta - (j+1)/r}).$$

The maximum in the exponent follows from Lemma 3.4, since

$$j \langle \beta - (j+1)/r = -1/r + [j \langle \beta - j/r] = -1/r + s_j,$$

where s_j is defined as in Lemma 3.4. This leads to the stated order (3.24) of the quadrature approximation. The case $l \leq \beta - r = m - 1$ follows immediately. For the second case, one can verify that

$$k + 1 - \frac{(k+1)\beta}{r} - \frac{1}{r} = -\frac{d+1}{r} + k + \frac{l - (m-1)}{r}$$

For r = 1, the second case does not arise because then $\beta = r + m - 1 = m$ and the condition $l \le m - 1$ always holds, so the result simplifies.

Thus far we proved the asymptotic error in approximating $I[f; h_x, P]$. The final result now follows from Corollary 3.1.

3.5 Numerical experiments

In this section we will illustrate the use of the method outlined in section §3.3 as well as the results regarding the asymptotic error behaviour predicted in Theorem 3.2.



Figure 3.3: Log-plot of error for different path approximations. Case of regular endpoint

3.5.1 Test of case with no stationary points

Consider the highly oscillatory integral

$$I[f] = \int_{-1}^{1} \sin(x) e^{i\omega/(x+2)} \mathrm{d}x$$

The oscillator g(x) = 1/(x+2) has no stationary points, meaning there are only contributions from the endpoints. The exact paths can be computed in this case.

In Figure 3.3 we have plotted the error of the two-point Gauss-Laguerre quadrature applied to the resulting line integrals with the given exact paths as well as approximate paths with different number of terms. Note that the approximate paths are constructed only with the knowledge of some derivatives of g.

The loss of order when using approximate paths, which can clearly be observed in Figure 3.3, is predicted in Theorem 3.2. We shall test the conclusion of the theorem by using approximate paths with different number of terms and different number of quadrature points, and then measuring the asymptotic order by regression for each combination. The result of this test can be seen in Table 3.1 along with the predicted order, $2n + 1 - 2n \setminus m$.

3.5.2 Comparison with classical asymptotic expansion

As noted in the introduction, the numerical method of steepest descent with approximated paths is asymptotic in its nature and should be compared to a classical

$n\downarrow,m\rightarrow$	exact	2	3	4	5
1	3.0(3)	2.0(2)	3.0(3)	3.0(3)	3.0(3)
2	5.0(5)	3.1(3)	4.0(4)	4.1(4)	5.0(5)
3	7.0(7)	4.2(4)	5.1(5)	6.9(6)	6.2(6)
4	9.0(9)	5.3(5)	7.1(7)	7.3(7)	8.0(8)

Table 3.1: Measured order for different numbers n of Gauss-Laguerre points with m termsin the Taylor expansion of the steepest-descent path. First column is with theexact path. Numbers in parentheses are orders predicted in Theorem 3.2.

	1 derivative of g			2 derivatives of g		
$\omega ightarrow$	10	50	100	10	50	100
Asymptotic	1.49e-02	1.24e-03	4.11e-05	2.10e-02	1.84e-04	2.85e-05
1-point NSD	1.53e-03	5.39e-04	3.27e-05	1.70e-02	1.56e-04	2.37e-05
2-point NSD	1.19e-03	2.98e-05	3.31e-06	3.96e-03	4.83e-07	1.85e-07
3-point NSD	1.01e-03	1.49e-06	7.59e-08	7.80e-04	1.87e-07	7.62e-09
4-point NSD	7.40e-04	5.48e-08	5.83e-10	3.07e-05	1.81e-08	2.25e-10

Table 3.2: Comparison of the error of the classical *n*-term asymptotic expansion which uses *n* derivatives of *g* and the *m*-term approximated path approximation which use m - 1 derivatives of *g*. The rows two to five contain results for numerical steepest descent with approximated paths and one to four quadrature points.

asymptotic expansion. This expansion, written out explicitly in eg. [16], requires derivatives of f, which the method of steepest descent does not. On the other hand, the asymptotic expansion only evaluates the functions at the endpoints, whereas the proposed method can be evaluated at a chosen number of complex evaluation points. A fair comparison is therefore not straightforward. We shall attempt this on applying the two approaches on the integral

$$I = \int_{-1}^{1} e^{i\omega\sin(\pi x/3)} \mathrm{d}x,$$

using $n = 1, \ldots, 4$ Gaussian evaluation points for the steepest descent method. The results in Table 3.2 shows that the method of steepest descent with approximated paths performs consistently better than the truncated asymptotic expansion. Note that adding evaluation points is computationally cheap; there is potential for doing much better with little extra work.

3.5.3 Case of stationary points

Now consider the integral

$$I = \int_0^1 \cos(x) e^{i\omega(x^3 + 2x^2)} \mathrm{d}x,$$

which has an order one stationary point at the origin. Even in this simple polynomial case the exact path originating from the stationary point is cumbersome to compute. Instead we construct the paths with the coefficients (3.15).

The steepest-descent integral corresponding to the path from the stationary point at x = 0 is computed with a scaled Gaussian quadrature. By using the exact path and a large number of quadrature points, we can nearly eliminate the error contribution from the right endpoint. Thus the error will be dominated by the error from the x = 0 contribution. Running over a range of different ω we estimate the order by regression, and the results fit with the predictions from Theorem 3.2 (see Table 3.3a).

No attempt to use exact paths at the origin was done, and the reference solution was obtained with Matlab's standard quadrature package close to machine precision.

For completion, we include the results from parallel tests done on the integral

$$I = \int_0^1 e^{i\omega(x^4 + 4x^3)} \mathrm{d}x,$$

which has an order 2 stationary point at the origin(Table 3.3b).

	$n\downarrow,m\rightarrow$	2	3	4
	1	1.0(1)	1.5(3/2)	1.5(3/2)
(a)	2	1.5(3/2)	1.5(3/2)	2.0(2)
	3	1.6(3/2)	2.4(5/2)	2.5(5/2)
	4	1.9(2)	2.4(5/2)	3.5(7/2)
	$n\downarrow,m\rightarrow$	2	3	4
	$\begin{array}{c} n\downarrow,m\rightarrow\\ 1\end{array}$	2 0.6(2/3)	3	4
(b)	$\begin{array}{c} n\downarrow,m\rightarrow\\ 1\\ 2 \end{array}$	2 0.6(2/3) 0.6(2/3)	3 1.0(1) 1.0(1)	4 1.0(1) 1.3(4/3)
(b)	$ \begin{array}{c} n \downarrow, m \rightarrow \\ 1 \\ 2 \\ 3 \end{array} $	2 0.6(2/3) 0.6(2/3) 0.9(1)	3 1.0(1) 1.0(1) 1.7(4/3)	4 1.0(1) 1.3(4/3) 1.3(4/3)

Table 3.3: Measured order for different numbers n of Gauss points with m terms in the expansion of the steepest-descent path. Numbers in parentheses are orders predicted in Theorem 3.2. a)-Case of order one stationary point, b)-Case of order two stationary point.



3.5.4 Effect of singularities on path approximations

Figure 3.4: Influence of singularities in the complex plane on the method. Error plotted for exact paths and path approximations with 2 and 4 terms



Figure 3.5: Contours of the imaginary part of the oscillator $g(x) = 1/(1+x^2)$ with exact path and approximations

It is important to note that the numerical method of steepest descent, both with exact and approximated paths, can perform well in non-analytical cases. Singularities in the complex plane have only an exponentially small influence on the integral. Of course, a quantity that is exponentially small for increasing ω may be arbitrarily large for any fixed value of ω and thus tangible restrictions on the size of ω may apply.

As an example we consider the integral

$$\int_0^1 e^{i\omega \frac{1}{1+x^2}} \mathrm{d}x$$

whose oscillator has poles at $x = \pm i$. By considering the asymptotics of the path equation (3.3), it is easy to verify that paths of steepest descent approach the poles as $p \to \infty$. If the paths are truncated they are contained in a section of the complex plane where the integrand is analytic and thus Cauchy's theorem applies. The pole at -i hardly affects the accuracy when using exact paths, as shown in Figure 3.4. However, the pole does affect the accuracy of the path approximation. The approximate paths using 2 or 4 terms are shown in Figure 3.5. Still, for ω large enough the influence of the pole is negated by the clustering of the evaluation points near the real axis. Using more evaluation points, some of which are located further away from the real axis, means that this effect comes in at a higher ω .

3.6 Extensions

In this final section we describe two extensions of the proposed scheme that are likely to be interesting in applications. We omit formal statements with proofs for the sake of brevity, but nevertheless we aim to be precise.

3.6.1 Avoiding the use of derivatives

	$n\downarrow,m\rightarrow$	2	3	4	5	
	1	2.0	3.0(3)	3.0(3)	3.0(3)	
(a)	2	3.1(3)	4.0(4)	4.1(4)	5.0(5)	
	3	4.2(4)	5.1(5)	7.0(6)	6.3(6)	
	4	5.7(5)	7.3(7)	7.7(7)	8.0(8)	
	$n\downarrow,m\rightarrow$	2		3	4	
(b)	1	1.0(1) 1.5	(3/2)	1.5(3/2)	
	2	1.5(3/	(2) 1.5	(3/2)	2.0(2)	
	3	1.4(3/	(2) 2.5	(5/2)	2.4(5/2)	
	4	1.8(2	2) 2.4	(5/2)	3.4(5/2)	

Table 3.4: Repetition of the experiments in Table 3.1 and 3.3(a), but with derivatives obtained from a finite difference approximation with appropriately scaled evaluation points.

The proposed scheme requires the computation of derivatives, which may not always be available. This is true for most numerical schemes for oscillatory integrals with high asymptotic order, because the asymptotic behaviour of the integral depends precisely on those derivatives. However, when aiming for high asymptotic order, it is sufficient to know derivatives only approximately, as long as the accuracy of the approximation scales with ω in a suitable fashion.

This was exemplified for Filon-type quadrature in [15]: Hermite interpolation of derivatives at critical points in this setting can be replaced by interpolation in points that are spaced $\mathcal{O}(\omega^{-1})$ apart without sacrificing asymptotic order of accuracy. A similar observation holds for our method: the exact derivatives of g can be replaced by finite difference approximations and it is sufficient that the points are spaced $\mathcal{O}(\omega^{-1})$ apart, and the asymptotic rate of error decay will stay the same.

To be precise, let us assume that the derivatives employed in the method are approximated with $O(\omega^{-1})$ error, i.e.,

$$\tilde{g}^{(k)}(x) = g^{(k)}(x) + e_k(\omega),$$
(3.32)

where $e_k(\omega) = \mathcal{O}(\omega^{-1})$. Note that when using finite differences of order h^p with $h \sim \omega^{-1}$ spacing, the error may actually be asymptotically smaller.

We construct path approximations h_x^* with coefficients \tilde{a}_j on the basis of these derivative approximations. One can verify that the $\mathcal{O}(\omega^{-1})$ error finds its way into the path equation with the same asymptotic size:

$$g(\tilde{h}_x^*(p)) = g(x) + ip + \sum_{k=r+m-1}^{\infty} \frac{(\sum_{j=1}^{\infty} \tilde{a}_j p^{j/r})^k}{k!} \tilde{g}^{(k)}(x) + E(\omega, p),$$

with $E(\omega, p) = \mathcal{O}(\omega^{-1})$ for each value of p.² Thus

$$g(\tilde{h}_{x}^{*}(q^{r})) = g(x) + iq^{r} + R_{r+m-1}(q) + E(\omega, q^{r}),$$

in the notation of §3.4.3. If we define a new residual function

$$\tilde{R}_{r+m-1}(q) = R_{r+m-1}(q) + E(\omega, q^r),$$

the proof of Theorem 3.2 must be reconsidered with this function. The critical point here is Lemma 3.3, which is concerned with the growth of derivatives of functions of the form $e^{\omega R_{\beta}}$. The property of vanishing derivatives (3.30) in this Lemma clearly doesn't hold for \tilde{R}_{β} . However, the derivatives are asymptotically small, i.e.,

$$\tilde{R}^{(j)}_{\beta}(0) = \mathcal{O}(\omega^{-1}), \quad 0 \le j < \beta.$$

With this condition replacing (3.30), the Lemma still holds. Thus mended, the proof in §3.4.4 in turn also holds.

Table 3.4 confirms this analysis. The experiments that were used in §5 to experimentally determine the order of the method are repeated here with simple finite difference approximations of the derivatives. The numbers are roughly the same as the numbers found in Tables 3.1 and 3.3(a).

²In order to see this, note that the coefficients \tilde{a}_j have an error of the same size regardless of the value of r, which follows for example from the explicit expressions in §3.

3.6.2 Two-dimensional integrals

Multivariate oscillatory quadrature is significantly more challenging than the univariate case. However, the benefits of exploiting high oscillation are also greater compared to traditional methods. The numerical method of steepest descent was extended to multivariate integrals in [13], based on repeated one-dimensional integration and tensor-product Gaussian quadrature. The computation of all steepestdescent paths involved is a delicate matter. It turns out that path approximations provide an important simplification in this procedure.

We consider a simple example to illustrate two-dimensional integration with approximated paths numerically. The integral

$$I[f] = \int_0^\infty \int_0^\infty e^{-x^2 - y^2} e^{i\omega \frac{1}{2x + y + 1}} dy dx$$

has only one contributing point, the origin. Treating it as an iterated integral requires us to solve for two paths of steepest descent, where the *inner path* for y depends on the outer integration variable x. The inner path u(p, x) satisfies

$$g(x, u(p, x)) = g(x, 0) + ip,$$
(3.33)

and the path v(q) for x is subsequently found from the equation

$$g(v(q),0) = g(0,0) + iq.$$
(3.34)

The combination leads to a steepest-descent manifold (u, v) which satisfies

$$g(v(q), u(p, v(q))) = g(0, 0) + ip + iq.$$

Construction of the paths simplifies considerably in the framework of approximated paths. For the experiment we fix the number of terms in the expansion of the two paths to be the same m. We solve equations (3.33) by replacing g(x, y)by its Taylor series in the y-direction and (3.34) by replacing g(x, 0) by its truncated Taylor series at the origin. These series are in turn inverted. Table 3.5 shows measured asymptotic order for a range of m, including exact paths, and number of evaluation points n, plus the accuracy the method achieves for this problem.

The measured rates of convergence in Table 3.5 appear to be exactly the same as those given in Table 3.1. Though an exact analysis of this case is more involved than the repeated application of the arguments used for the univariate case, this result should not be surprising as one can indeed think of the double integral as a repeated one-dimensional integral with approximate paths, each of which has a known asymptotic behaviour.

This line of thinking does not generalize however to the case of stationary points, where the gradient of the oscillator vanishes, and the case of resonance points, where the gradient of the oscillator is orthogonal to the tangent of the integration domain's boundary. Both generalizations are a topic of further research. The simplicity of path approximations, with explicit expressions for the path approximations, presents a motivating factor for this research.

	$n\downarrow,m\rightarrow$	exact	2	3	4	5
-	1	3.0	2.0	3.0	3.0	3.0
a)	2	5.0	3.0	4.0	4.0	5.0
	3	7.0	4.1	4.9	6.1	6.0
	4	9.3	5.3	6.9	7.0	8.4
	$n\downarrow,\omega\rightarrow$	10		50		100
	1	1.05e-02	4.	01e-04	1.0	0e-04
b)	2	4.11e-03	1.	72e-05	2.0)4e-06
	3	4.25e-03	1.	30e-06	6.5	8e-08
	4	3.74e-03	1.	52e-07	3.1	0e-09

Table 3.5: a) Measured order for different numbers n of Gauss-Laguerre points with mterms in the Taylor expansion of the steepest-descent paths for a 2D-example.First column is with the exact path.b) Absolute error for the approximationobtained with two-term path approximations.

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Paper III

Local solutions to high frequency scattering problems

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Chapter 4

Local solutions to high frequency scattering problems

Abstract. We consider the solution of high-frequency scattering problems in two dimensions, modeled by an integral equation on the boundary of a smooth scattering object. We devise a numerical method to obtain solutions on only parts of the boundary with little computational effort. The method incorporates asymptotic properties of the solution and can therefore attain particularly good results for high frequencies. We show that the integral equation in this approach reduces to an ordinary differential equation.

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