

# NUMERICAL INTEGRATION OF FUNCTIONS OF A RAPIDLY ROTATING PHASE

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ABSTRACT. We present an algorithm for the efficient numerical evaluation of integrals of the form

$$I(\omega) = \int_0^1 F(x, e^{i\omega x}; \omega) dx$$

for sufficiently smooth but otherwise arbitrary  $F$  and  $\omega \gg 1$ . The method is entirely “black-box”, i.e., does not require the explicit computation of moment integrals or other pre-computations involving  $F$ . Its performance is uniform in the frequency  $\omega$ . We prove that the method converges exponentially with respect to its order when  $F$  is analytic and give a numerical demonstration of its error characteristics.

## 1. INTRODUCTION

We consider the problem of numerical approximation of integrals of the form

$$I(\omega) = \int_0^1 F(x, e^{i\omega x}; \omega) dx, \tag{1}$$

where  $F: [0, 1] \times \mathbb{U} \rightarrow \mathbb{C}$ ,  $\mathbb{U}$  denotes the unit circle in the complex plane, and  $\omega > 0$ .  $F$  may, in addition, depend parametrically on  $\omega$ . In most of the following, we will not write out this parametric dependence explicitly except where it matters for a precise statement of the quadrature error estimate. Classical quadrature formulas require that the number of integration nodes grows linearly in the frequency  $\omega$ , so that the problem becomes increasingly intractable when the frequency is large.

One of the earliest integration methods for integrals of this type is due to Filon [7], who studied the special case

$$F(x, e^{i\omega x}; \omega) = F(x, e^{i\omega x}) = f(x) e^{i\omega x}. \tag{2}$$

Filon replaced the function  $f$  by a polynomial approximation so that the resulting moment integrals could be computed analytically. The method has been refined and extended by many authors [8, 21, 23]. Other methods use interpolatory formulas and formulas which are based on the integration between the zeros of  $\cos(\omega x)$  and  $\sin(\omega x)$  [14, 15, 20].

Most subsequent work went into oscillatory integrals of the form

$$I(\omega) = \int_0^1 f(x) e^{i\omega g(x)} dx \tag{3}$$

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which is a more subtle problem when the phase function  $g$  has stationary points. Levin [13] suggested to convert the integrand into a perfect derivative. He seeks a function  $p$  satisfying

$$\frac{d}{dx}(p(x)e^{i\omega g(x)}) = f(x)e^{i\omega g(x)}, \quad (4)$$

a differential equation which can be solved by collocation. The value for the integral is then recovered via

$$I(\omega) = \int_0^1 f(x)e^{i\omega g(x)} dx = p(1)e^{i\omega g(1)} - p(0)e^{i\omega g(0)}. \quad (5)$$

Olver [18] suggest a choice of approximation basis for  $f$  which is compatible with integration against  $e^{i\omega g(x)}$  so that Filon-type ideas can be extended to problem (3).

A third approach is based on asymptotic expansion in inverse powers of the frequency. It can be shown that

$$I(\omega) = \sum_{k=0}^{p-1} \frac{1}{(-i\omega)^{k+1}} \left( \frac{e^{i\omega g(1)}}{g'(1)} f_m(1) - \frac{e^{i\omega g(0)}}{g'(0)} f_m(0) \right) + O(\omega^{-p-1}) \quad (6)$$

with

$$f_0(x) = f(x) \quad \text{and} \quad f_{m+1}(x) = \frac{d}{dx} \frac{f_m(x)}{g'(x)}, \quad (7)$$

so that the sum on the right of (6) provides an accurate approximation when  $\omega$  is large. Iserles and Nørsett [11, 12] modify (6) as to not require the computation of derivatives at the endpoint while producing errors comparable to other asymptotic and Filon-type methods. For reviews of available methods and further references, see [6, 10].

None of the methods mentioned so far, however, extends to (1) in the general case, i.e., without exploiting a particular form of the function  $F$ . We encountered integrals of this form when extending uniformly accurate exponential integrators for the Klein–Gordon equation in the non-relativistic limit, first suggested by Baumstark *et al.* [4], to problems with more general nonlinearities [16].

In this paper, we derive a uniformly accurate quadrature scheme that is completely “black-box”, i.e., can be applied to any function  $F$  without  $F$ -specific pre-computations. It is based on Gauss quadrature for sums detailed in Section 2 below. We show that the quadrature error is exponentially small in  $n$  when  $F$  is analytic.

To motivate our approach, let  $T = 2\pi/\omega$  denote the period of  $x \mapsto e^{i\omega x}$ . Then there exist  $N \in \mathbb{N}$  and  $\alpha \in [0, 1)$  such that

$$(N + \alpha)T = 1. \quad (8)$$

Let now  $x_j$  be the  $N + 1$  equidistant points

$$x_j = -1 + \frac{2j}{N-1}, \quad 0 \leq j \leq N. \quad (9)$$

We can write

$$\begin{aligned}
 I(\omega) &= \sum_{j=0}^{N-1} \int_{jT}^{(j+1)T} F(x, e^{i\omega x}) dx + \int_{NT}^{(N+\alpha)T} F(x, e^{i\omega x}) dx \\
 &= T \sum_{j=0}^{N-1} \int_0^1 F(T(t+j), e^{2\pi it}) dt + T \int_0^\alpha F(T(t+N), e^{2\pi it}) dt \\
 &= T \sum_{j=0}^{N-1} I_1(x_j) + T I_\alpha(x_N)
 \end{aligned} \tag{10}$$

with

$$I_b(y) = \int_0^b F(Tt + \frac{1}{2}T(N-1)(y+1), e^{2\pi it}) dt. \tag{11}$$

When  $F$  depends parametrically on  $\omega$ ,  $I_b$  inherits this parametric dependence. Importantly, (11) shows that  $I_b(y)$  is otherwise independent of  $\omega$  so that, for fixed  $y$ , each  $I_b(y)$  can be evaluated easily via any traditional quadrature rule; errors are uniform in  $\omega$  as all derivatives of the integrand are uniform in  $\omega$ . Moreover,  $I_1(y)$  varies slowly as a function of  $y$ . Thus, the sum on the right hand side of (10) could be seen as a Riemann sum,

$$2T \sum_{j=0}^{N-1} I_1(x_j) = \int_{-1}^1 I_1(y) dy + O(\omega^{-1}), \tag{12}$$

where the right hand integral could, again, be approximated by any traditional quadrature rule. Since  $NT < 2\pi$ , the integrand in the definition of  $I_1(y)$ , see (11), has uniformly bounded derivatives with respect to both  $t$  and  $y$  as  $N \rightarrow \infty$ , equivalently  $\omega \rightarrow \infty$ , so that the error behavior of any traditional quadrature rule remains uniform in this limit.

The resulting method would be efficient and has an error that is asymptotically small for large  $\omega$ . However, it turns out that we can do even better, by-passing the Riemann sum approximation (12) with its  $O(\omega^{-1})$ -error entirely: Sums with a slowly varying summand can be evaluated effectively via Gauss quadrature for sums with a small number of evaluations, just like Gauss quadrature for integrals. Gauss quadrature for sums has been described by Area *et al.* [2, 3] but, to the best of our knowledge, has never been applied in the context of oscillatory integrals.

The remainder of the paper is structured as follows. Gauss quadrature for sums is detailed in Section 2, leading to a complete statement of the algorithm. Section 3 gives a simple estimate for the quadrature error. Finally, in Section 4, we demonstrate that the method is easy to implement and performs well.

## 2. GAUSS QUADRATURE FOR SUMS

Let  $N$  be a positive integer, arbitrary but fixed; for ease of notation, we shall omit any implicit dependence on  $N$  in the following. Then there exists a unique quadrature formula

$$S(G) \equiv \frac{2}{N} \sum_{j=0}^{N-1} G(x_j) \approx \sum_{k=1}^n w_k G(s_k) \equiv S_n(G), \tag{13}$$

which is exact for all polynomials of degree  $\leq 2n - 1$ . In our context,  $N = O(\omega)$  is typically very large. If  $G$  is sufficiently smooth—see Section 3 below for precise statements—the number of terms  $n$  on the right-hand side can still be very small. In practice,  $n = 4$  already gives very accurate results and improvements above  $n = 8$  are mostly limited by floating point error, see Section 4. Crucially, the error depends only on the properties of  $G$ , not on the number of terms in the left-hand sum  $N$ . Thus, it is uniform as  $N \rightarrow \infty$ .

The construction uses so-called Gram polynomials  $p_m$ ,  $m = 0, \dots, N - 1$ , which are defined, up to choice of sign, by their orthonormality with respect to a discrete equidistant sum, namely

$$\sum_{j=0}^{N-1} p_l(x_j) p_m(x_j) = \delta_{lm}. \quad (14)$$

Here, we follow the terminology of [5]. The Gram polynomials are also known as discrete Chebyshev polynomials and appear as special cases in the more general family of Hahn polynomials; see, e.g., [1] for a discussion.

For fixed  $n < N$ , the quadrature nodes  $\{s_k\}$  are the zeros of the Gram polynomial of degree  $n$ . Then

$$q_k(x) = \frac{p_n(x)}{x - s_k} - \frac{a_n}{a_{n-1}} p_{n-1}(x) \quad (15)$$

is a polynomial of degree  $n - 2$ , where  $a_m$  denotes the leading coefficient of  $p_m$ .

For any polynomial  $p$  of degree  $\leq 2n - 1$  that vanishes at all the nodes  $s_l$  except for  $s_k$ , (13) implies that

$$w_k = \frac{2}{N p(s_k)} \sum_{j=0}^{N-1} p(x_j). \quad (16)$$

Taking

$$p(x) = \frac{p_n(x) p_{n-1}(x)}{x - s_k}, \quad (17)$$

in particular, we obtain

$$w_k = \frac{2}{N p'_n(s_k) p_{n-1}(s_k)} \sum_{j=0}^{N-1} \frac{p_n(x_j) p_{n-1}(x_j)}{x_j - s_k}. \quad (18)$$

Since  $q_k$  is of degree  $n - 2$ , it is orthogonal to  $p_{n-1}$ . We conclude that

$$w_k = \frac{a_n}{a_{n-1}} \frac{2}{N p'_n(s_k) p_{n-1}(s_k)}. \quad (19)$$

The Gram polynomials  $p_n$  can be expressed in closed form in terms of the hypergeometric function  ${}_3F_2$  by

$$p_n(x) = (-1)^n \sqrt{\frac{(2n+1)(N-n)_n}{(N)_{n+1}}} {}_3F_2 \left( \begin{matrix} -n, & n+1, & (1-N)(1+x)/2 \\ & 1, & 1-N \end{matrix} \middle| 1 \right), \quad (20)$$

[9, Equations 7.13.7 and 7.13.15], with Pochhammer symbol defined by

$$(A)_0 = 1, \quad (A)_n = A(A+1)(A+2) \cdots (A+n-1) \text{ for } n \in \mathbb{N}^*. \quad (21)$$

By expanding the finite series representation of  ${}_3F_2$ , we find that the leading order coefficient is given by

$$a_n = \sqrt{\frac{(2n+1)(N-n-1)!}{(N+n)!} \frac{(2n)!(N-1)^n}{2^n (n!)^2}} \quad (22)$$

so that

$$\frac{a_n}{a_{n-1}} = \frac{N-1}{n} \sqrt{\frac{4n^2-1}{N^2-n^2}}. \quad (23)$$

For details, see [9, p. 348] and [17, p. 170]. We note that the expressions in [2, 3] differ from the ones given here due to the different choice of nodes in the definition of the discrete inner product in (14).

Applying the Gauss summation formula (13) to (10), we obtain the final quadrature approximation

$$I_{\text{comp}}(\omega; n) = \frac{NT}{2} \sum_{k=1}^n w_k I_1(s_k) + T I_\alpha(x_N). \quad (24)$$

### 3. CONVERGENCE ANALYSIS

In the following, we use the Chebyshev approximation to quantify the error of the Gauss quadrature formula for sums. To fix notation, let  $G$  be a continuous function on  $[-1, 1]$ . We write

$$G_n(x) = \sum_{j=0}^n a_j T_j(x) \quad (25)$$

to denote its polynomial approximation of degree  $n$  obtained by truncating the Chebyshev series at order  $n$ . Here,  $T_j(x) = \cos(j \arccos(x))$  is the Chebyshev polynomial of degree  $j$  and the coefficients are given by

$$a_0 = \frac{1}{\pi} \int_{-1}^1 \frac{G(x)}{\sqrt{1-x^2}} dx, \quad (26a)$$

$$a_j = \frac{2}{\pi} \int_{-1}^1 \frac{G(x) T_j(x)}{\sqrt{1-x^2}} dx \text{ for } j \geq 1. \quad (26b)$$

We write  $\|\cdot\|$  to denote the supremum norm on  $[-1, 1]$  and define

$$d_n = \|G - G_n\|. \quad (27)$$

**Proposition 1.** *Let  $G \in \mathcal{C}([-1, 1])$  and  $S$  and  $S_n$  be defined as in (13). Then*

$$|S(G) - S_n(G)| \leq 4 d_{2n-1}. \quad (28)$$

*Proof.* As (13) is exact for polynomials of degree  $\leq 2n-1$ , we have  $(S - S_n)(G) = (S - S_n)(G - G_{2n-1})$ . Hence,

$$\begin{aligned} |S(G) - S_n(G)| &\leq |S(G - G_{2n-1})| + |S_n(G - G_{2n-1})| \\ &\leq 2 d_{2n-1} + \sum_{k=1}^n |w_k| d_{2n-1}. \end{aligned} \quad (29)$$

Since the weights are non-negative [17] and formula (13) is interpolatory,

$$\sum_{k=1}^n |w_k| = 2 \quad (30)$$

which implies (28).  $\square$

When  $G$  is smooth, the error of the Chebyshev approximation satisfies the following strong bounds.

**Theorem 2** ([22, Theorem 4.3]). *Let  $G \in \mathcal{C}([-1, 1])$  be such that  $G, G', \dots, G^{(m-1)}$  are absolutely continuous and*

$$\left\| \frac{G^{(m)}}{\sqrt{1-x^2}} \right\|_1 \equiv V < \infty \quad (31)$$

for some  $m \geq 1$ . Then, for every  $n \geq m + 1$ ,

$$d_n \leq \frac{2V}{\pi m (n-m)^m}. \quad (32)$$

Moreover, if  $G$  is analytic with  $|G(z)| \leq M$  in the region bounded by the ellipse with foci  $\pm 1$  and major and minor semiaxis lengths summing to  $\rho > 1$ , then for every  $n \geq 0$ ,

$$d_n \leq \frac{2M}{(\rho-1)\rho^n}. \quad (33)$$

Applying Proposition 1 and Theorem 2 to the function  $G(y) = I_1(y; \omega)$  directly yields the following error estimate for the outer quadrature.

**Theorem 3.** *Fix  $\omega_0 \geq 4\pi$  and  $m \in \mathbb{N}$ . Let  $F: [0, 1] \times \mathbb{U} \rightarrow \mathbb{C}$  be continuous. Assume further that the  $m-1$  first derivatives of  $I_1(y; \omega)$  defined in (11) are absolutely continuous on  $[-1, 1]$  and that there exists a constant  $V$  such that*

$$\left\| \frac{I_1^{(m)}(\cdot; \omega)}{\sqrt{1-y^2}} \right\|_1 \leq V \quad (34)$$

uniformly with respect to  $\omega \geq \omega_0$ . Then, for every  $n \geq m/2 + 1$ ,

$$\left| I(\omega) - \frac{NT}{2} \sum_{k=1}^n w_k I_1(s_k) - I_\alpha(x_N) \right| \leq \frac{4V}{m(2n-1-m)^m}. \quad (35)$$

Moreover, if  $I_1(y)$  is analytic with  $|I_1(y)| \leq M$  in the region bounded by the ellipse with foci  $\pm 1$  and major and minor semiaxis lengths summing to  $\rho > 1$ , uniformly in  $\omega \geq \omega_0$ , then for every  $n \geq 1$ ,

$$\left| I(\omega) - \frac{NT}{2} \sum_{k=1}^n w_k I_1(s_k) - I_\alpha(x_N) \right| \leq \frac{4M}{(\rho-1)\rho^{2n-1}}. \quad (36)$$

*Remark 4.* The assumption  $\omega_0 \geq 4\pi$  ensures that  $N \geq 2$  so that the Gram polynomials are well defined. When  $\omega < 4\pi$ ,  $x \mapsto F(x, e^{i\omega x})$  is not highly oscillatory so that classical methods are applicable.

*Remark 5.* It is possible to formulate sufficient conditions which directly refer to  $F$ . Since

$$\begin{aligned} \left\| \frac{I_1^{(m)}}{\sqrt{1-y^2}} \right\|_1 &\leq \frac{1}{2^{m+1}\pi} \int_{-1}^1 \int_0^{2\pi} \frac{|\partial_x^m F(\omega^{-1}s + \frac{1}{2}T(N-1)(y+1), e^{is}; \omega)|}{\sqrt{1-y^2}} ds dy \\ &\leq \frac{\pi}{2^m} \sup_{x,z} |\partial_x^m F(x, z; \omega)|, \end{aligned} \quad (37)$$

estimate (35) holds whenever the first  $m$   $x$ -derivatives of  $F$  are uniformly bounded with respect to  $x$ ,  $z$ , and  $\omega$ . Likewise, estimate (36) holds whenever  $F$  is analytic in its first argument with a radius of analyticity that is uniform with respect to  $x$ ,  $z$ , and  $\omega$ . However, Theorem 3 as stated is stronger because  $I_1(y; \omega)$  may be uniformly analytic even if  $F$  is not uniformly analytic in its first argument, as the example given in the next section shows. Moreover, estimate (37) for  $V$  and analogous estimates for  $M$  will generally over-estimate the constants.

In the discussion above, we have not specified a quadrature rule for the “inner integrals” (11). The choice of scheme and resulting inner quadrature error depends on the smoothness of  $F$  in both arguments (in fact, more strongly on the second). Since the inner quadrature is always over a full period of sine and cosine functions, the required number of quadrature points is typically larger, but not excessively larger, than the number of quadrature nodes for the outer sum. In the following, we illustrate the error behavior with concrete numerical examples. In particular, we show that the outer quadrature can be well-behaved even if the inner quadrature is nearly singular. Even then, our outer scheme combined with an off-the-shelf library routine for the inner scheme performs uniformly well as  $\omega$  grows large.

#### 4. IMPLEMENTATION AND NUMERICAL TEST

We consider the example

$$F(x, e^{i\omega x}; \omega, a) = \frac{2x - \omega \sin(\omega x)}{2\sqrt{a + x^2 + \cos(\omega x)}} \quad (38)$$

with  $a \geq 1$ . Here, standard quadrature libraries fail or perform increasingly poorly when  $\omega$  becomes large. On the other hand, the exact value of the integral can be computed directly, it is

$$I_{\text{exact}}(\omega; a) = \sqrt{a + 1 + \cos(\omega)} - \sqrt{a + 1}. \quad (39)$$

Moreover, the inner integral (11) can also be computed explicitly:

$$\begin{aligned} I_1(y; \omega, a) &= \frac{1}{4\pi} \int_0^{2\pi} \frac{2\pi(N-1)(y+1) + 2s - \omega^2 \sin(s)}{\sqrt{a\omega^2 + (\pi(N-1)(y+1) + s)^2 + \omega^2 \cos(s)}} ds \\ &= \frac{2\pi((N-1)y + N)}{\sqrt{(a+1)\omega^2 + \pi^2(N-1)^2(y+1)^2} + \sqrt{(a+1)\omega^2 + \pi^2((N-1)y + N + 1)^2}}. \end{aligned} \quad (40)$$

Since  $\omega \sim 2\pi N$ ,

$$\lim_{\omega \rightarrow \infty} I_1(y; \omega, a) = \frac{y+1}{\sqrt{4(a+1) + (y+1)^2}}, \quad (41)$$

so that  $I_1$  is uniformly analytic. Thus, estimate (36) of Theorem 3 provides an error bound for the *outer* quadrature that is uniform in  $\omega$ . Via the limiting expression, we can even get a quantitative lower bound on the scaling exponent: the right hand side of (41) has poles at  $z = -1 \pm 2i\sqrt{a+1}$  and we need to find the radius  $\rho$  of the circle in the complex plane such that its image under  $z \mapsto (z + z^{-1})/2$ , the Bernstein ellipse, touches the poles. A routing application of a root finding scheme yields  $\rho_{\text{theor}} = 7.33$  when  $a = 2$ . For the actual quadrature error of our method, we obtain a best fit scaling exponent  $\rho_{\text{num}} \approx 8.96$  (Figure 1, dotted line). Thus, the actual scheme scales slightly better, but (36) is not far off and provides a consistent upper bound.

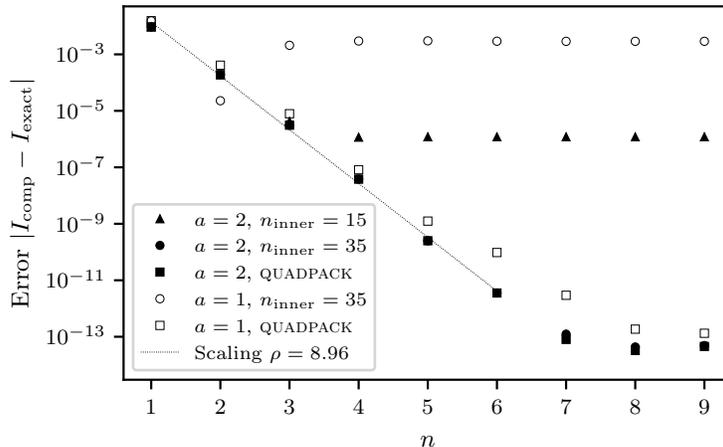


FIGURE 1. Scaling of the error with the number of the outer Gauss quadrature nodes  $n$ . We compare different schemes for the inner quadrature for the case when  $F$  is uniformly analytic ( $a = 2$ , filled marker symbols) with the case when uniform analyticity fails and non-adaptive inner Gauss–Legendre quadrature struggles ( $a = 1$ , empty marker symbols). In this example,  $\omega = 10^4$  is fixed.

The error behavior of the *inner* quadrature depends on the choice of  $a$ . When  $a = 1$ , the right hand side of (38) has four poles

$$x = \pm \frac{\pi}{\omega} \pm \frac{i\sqrt{2}\pi}{\omega^2} + O(\omega^{-3}) \quad (42)$$

that approach the interval of integration on the real axis as  $\omega \rightarrow \infty$ . As shown above, these poles do not affect the outer quadrature (except that the simplified sufficient conditions of Remark 5 are not applicable in this case). However, they do affect the behavior of the inner quadrature: In a small region near  $s = \pi$ , corresponding to  $t = 1/2$ , the inner integrand develops steep gradients as  $\omega$  becomes large; correspondingly, error estimates for Gauss–Legendre quadrature based, e.g., on Chebyshev approximation as in Theorem 2, break down in this limit. This behavior is seen clearly in the numerical test where Gauss–Legendre quadrature of fixed order performs poorly on the inner integral (Figure 1, open circles). Nonetheless, standard adaptive quadrature implementations have no difficulty dealing with this case and perform well. In our example implementation, we use a binding to the well known Fortran library QUADPACK [19] (Figure 1, open squares).

For any  $a > 1$ , the poles of the expression on the right of (38) remain a uniform distance away from the interval of integration. We show results for  $a = 2$  where the inner integral can be calculated effectively by a moderate order classical Gauss–Legendre quadrature:  $n_{\text{inner}} \geq 35$  gives errors comparable to errors achievable with QUADPACK (Figure 1, filled markers).

Figure 2 illustrates the uniformity of the error as a function of  $\omega$ .

We note that the Gauss summation nodes  $s_k$  and weights  $w_k$  depend on  $\omega$ , so they must be re-computed whenever  $\omega$ , hence  $N$ , is changed. The Gram polynomials

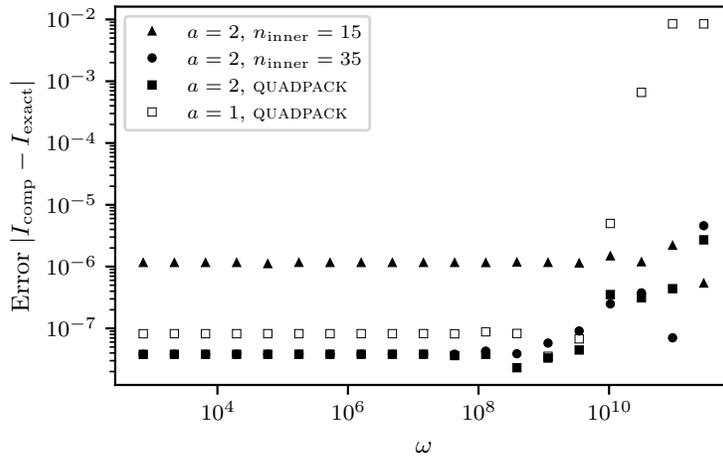


FIGURE 2. Demonstration of the uniformity of the Gauss summation scheme with respect to the fast frequency  $\omega$ . For very large values of  $\omega$ , accuracy is necessarily lost due to the loss of significant digits in the evaluation of the trigonometric functions in double-precision floating point. In this example, the number of outer Gauss quadrature nodes is fixed at  $n = 4$ .

themselves are polynomials of degree  $n$  with coefficients which, up to normalization, are polynomials in  $N$  of degree  $n$ . Thus, the polynomial data can be pre-computed and stored in an integer array of size  $n^2$  and evaluated in  $O(n^2)$  operations. The roots are found with the Weierstrass–Dochev–Durand–Kerner algorithm which is known to converge rapidly for Gram polynomials [3]. Since the classical Gauss–Legendre quadrature points—the continuum limit of Gauss summation—provide a good initial guess, this algorithm reaches excellent accuracy in a small number of iterations which is uniform in  $N$ . Moreover, all  $N$ -dependent terms need to be evaluated only once, so that the overall complexity of the root finding step remains at  $O(n^2)$ . In our example implementation, provided as supplementary material to the manuscript, we use a symbolic mathematics package for all polynomial manipulations. This adds some run-time overhead but leads to a transparent and still reasonably fast implementation.

The complexity of the overall quadrature formula is the complexity of the evaluation of the weights, which can be done at  $O(n^2)$  as all  $N$ -dependent terms need to be evaluated only once, times  $n_{\text{inner}}$ , the complexity of the inner quadrature, which is problem-dependent as discussed above. If several integrals with the same frequency  $\omega$  are performed, the quadrature weights can be precomputed and the complexity per evaluation drops to  $O(n \cdot n_{\text{inner}})$ . Also, the required number of function evaluations is always  $n \cdot n_{\text{inner}}$ . Since, in many cases, order  $n = 6$  is already very accurate and order  $n = 10$  is mainly limited by floating point error, and provided the inner integration is sufficiently well-behaved, the method is very effective in practice.

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