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Preconditioned GMRES for oscillatory integrals

Sheehan Olver

Oxford University Computing Laboratory, Wolfson Building, Parks Road, Oxford, UK

Sheehan.Olver@sjc.ox.ac.uk

Abstract None of the existing methods for computing the oscillatory integral $\int_a^b f(x)e^{i\omega g(x)}\,dx$ achieve all of the following properties: high asymptotic order, stability, avoiding the computation of the path of steepest descent and insensitivity to oscillations in f. We present a new method that satisfies these properties, based on applying the GMRES algorithm to a preconditioned differential operator.

Keywords GMRES, highly oscillatory integrals, asymptotics.

Oxford University Computing Laboratory
Numerical Analysis Group
Wolfson Building
Parks Road
Oxford, England OX1 3QD

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1. Introduction

Consider the oscillatory integral

$$I[f] = \int_a^b f(x) e^{i\omega g(x)} \, dx,$$

where f and g are $\mathbb{C}^\infty[\Omega]$ and g' does not approach zero in Ω, where $\Omega = \mathrm{cl}\,(a,b)$. We construct a new method $Q_n^{\mathcal{M}}[f]$ with the following properties:

(1) The method achieves the asymptotic order

$$I[f] - Q_n^{\mathcal{M}}[f] = \mathcal{O}\left(\omega^{-n-1}\right), \qquad \omega \to \infty;$$

(2) For sufficiently large ω, the method is guaranteed to converge as $n \to \infty$ for a large class of analytic functions f and g, based on the growth of $\frac{f(g^{-1}(t))}{g'(g^{-1}(t))}$ in the complex plane (though g^{-1} is not needed in the algorithm itself);

(3) For fixed n, $Q_n^{\mathcal{M}}[f]$ is numerically stable for sufficiently large ω;

(4) $Q_n^{\mathcal{M}}[f]$ can be applied to integrals over unbounded intervals;

(5) If $f = r e^{ikp}$ and p' does not approach zero in Ω, then the error remains small as k increases, without needing to know the form of p or r;

(6) The method is still accurate when ω is complex.

Many advances have been made recently for the computation of $I[f]$; for example, Filon-type methods [**5**], moment-free Filon-type methods [**11**], Levin-type methods [**10**] and numerical steepest descent [**4**]. Each of these methods achieves the first property whilst none of these methods achieve the fifth property. Moreover, Filon-type methods are only applicable for certain oscillators, in particular oscillators for which the moments

$$\int_a^b x^k e^{i\omega g(x)} \, dx$$

are known. A numerical stable algorithm for computing a Filon-type method is only known for $g(x) = x$. Moment-free Filon-type methods avoid computation of moments, but they are not numerically stable as constructed in [**11**]. We know that Filon-type methods converge due to the uniform convergence of polynomial interpolation at Chebyshev points [**12**]. Whether this holds true for moment-free Filon-type methods is unknown. Because these methods are based on polynomial interpolation, they can not be applied to integrals over unbounded intervals. Though a numerically stable algorithm exists for computing the Levin collocation method [**6**], it cannot be used to achieve high asymptotic orders, which requires solving an ill-conditioned collocation system.

Numerical steepest descent is stable, and achieves a higher asymptotic order than any other method using the same amount of information. Unfortunately, it requires deforming the path of integration into the complex plane, which is not always possible, and even when it is possible, complications arising from singularities, branch cuts, and supergeometric growth in the complex plane can prevent convergence, or be a logistical nightmare to resolve. Furthermore, for a fixed number of sample points, the error blows up as $\omega \to 0$, so an alternative quadrature scheme is necessary in the nonoscillatory regime.

Suppose $v \in \mathbb{C}^\infty[\Omega]$ is a particular solution to the Levin differential equation

$$\mathcal{L}v = f, \qquad \text{for} \qquad \mathcal{L} = \mathcal{D} + \mathrm{i}\omega g'. \tag{1.1}$$

Finding a solution to this differential equation allows us to evaluate the integral as

$$I[f] = \int_a^b \mathrm{e}^{\mathrm{i}\omega g} \mathcal{L}v \,\mathrm{d}x = \int_a^b (v\mathrm{e}^{\mathrm{i}\omega g})' \,\mathrm{d}x = v(b)\mathrm{e}^{\mathrm{i}\omega g(b)} - v(a)\mathrm{e}^{\mathrm{i}\omega g(a)}.$$

Thus approximating a solution to (1.1) allows us to approximate $I[f]$. The Levin collocation method solves (1.1) using a collocation system without boundary conditions [**7**], and Levin-type methods used derivative information at the endpoints to achieve higher asymptotic orders [**10**].

As an alternative, we will use GMRES on the differential operator to compute the solution (1.1), a process which we refer to as diffferential GMRES. Define the Krylov subspace

$$\mathcal{K}_n[\mathcal{L}, f] = \operatorname{span}\left\{f, \mathcal{L}f, \mathcal{L}^2 f, \ldots, \mathcal{L}^{n-1} f\right\}.$$

Given a semi-inner product $\langle \cdot, \cdot \rangle$, the GMRES algorithm finds a function $v_n^{\mathcal{L}} \in \mathcal{K}_n[\mathcal{L}, f]$ which minimizes the residual $\left\| f - \mathcal{L}v_n^{\mathcal{L}} \right\|$, where $\|\cdot\| = \sqrt{\langle \cdot, \cdot \rangle}$. We can then approximate $I[f]$ by

$$Q_n^{\mathcal{L}}[f] = v_n^{\mathcal{L}}(b)\mathrm{e}^{\mathrm{i}\omega g(b)} - v_n^{\mathcal{L}}(a)\mathrm{e}^{\mathrm{i}\omega g(a)}.$$

Remark: Unless otherwise stated, $\langle \cdot, \cdot \rangle$ denotes a general semi-inner product (independent of ω) on some vector space V with seminorm $\|\cdot\| = \sqrt{\langle \cdot, \cdot \rangle}$, $\langle \cdot, \cdot \rangle_2$ is the L_2 inner product over Ω with Legendre weight and $\|\cdot\|_p$ is the L_p norm with Legendre weight, or, when applied to a vector, the ℓ_p vector norm. For a complex set S, we use the notation $\|\cdot\|_S$ to denote the supremum norm over S, thus $\|\cdot\|_\Omega$ and $\|\cdot\|_\infty$ are equivalent. We also use the semi-norm

$$\langle\!\langle q, r \rangle\!\rangle_m = \sum_{k=1}^m w_k q(x_k) \bar{r}(x_k),$$

where the weights are nonzero, $x_1 = a$ and $x_m = b$. In the examples, we use either $\langle \cdot, \cdot \rangle_2$ or $\langle\!\langle \cdot, \cdot \rangle\!\rangle_m$ with Clenshaw–Curtis weights and nodes when Ω is bounded. When a is finite and

b is infinite, we use the Laguerre inner product

$$\langle f, g \rangle_L = \int_a^\infty f \bar{g} \mathrm{e}^{-x} \, \mathrm{d}x.$$

Note that $\mathcal{K}_n[\mathcal{L}, f] = \mathcal{K}_n\Big[\mathcal{D}, f\mathrm{e}^{\mathrm{i}\omega g}\Big] \, \mathrm{e}^{-\mathrm{i}\omega g}$, and the method just described is equivalent to the differential GMRES method from [**13**], where GMRES was applied to the differentiation operator $\mathcal{D}$. In that paper it was observed that differential GMRES has an asymptotic order

$$I[f] - Q_n^{\mathcal{L}}[f] = \mathcal{O}\Big(\omega^{-n-1}\Big)\,, \qquad \omega \to \infty,$$

when the kernel of oscillations is a standard Fourier oscillator ($g(x) = x$). In this paper we will show that the same convergence rate can be obtained for more general oscillators g by using preconditioning. Define the operator

$$\mathcal{M} = \mathcal{L}\frac{1}{g'} = \mathcal{D}\frac{1}{g'} + \mathrm{i}\omega.$$

Note that

$$\int_a^b \mathrm{e}^{\mathrm{i}\omega g} \mathcal{M} v \, \mathrm{d}x = \int_a^b \mathrm{e}^{\mathrm{i}\omega g} \mathcal{L} \frac{v}{g'} \, \mathrm{d}x = \frac{v(b)}{g'(b)} \mathrm{e}^{\mathrm{i}\omega g(b)} - \frac{v(a)}{g'(a)} \mathrm{e}^{\mathrm{i}\omega g(a)};$$

hence solving $\mathcal{M}v = f$ also allows us to compute $I[f]$. Let $v_n^{\mathcal{M}} \in \mathcal{K}_n[\mathcal{M}, f]$ be the function produced by GMRES which minimizes the seminorm of the residual $\Big\| f - \mathcal{M} v_n^{\mathcal{M}} \Big\|$. We then obtain the following approximation to $I[f]$:

$$Q_n^{\mathcal{M}}[f] = \frac{v_n^{\mathcal{M}}(b)}{g'(b)} \mathrm{e}^{\mathrm{i}\omega g(b)} - \frac{v_n^{\mathcal{M}}(a)}{g'(a)} \mathrm{e}^{\mathrm{i}\omega g(a)}.$$

To ensure this definition makes sense, we assume throughout the paper that $\frac{p(b)}{g'(b)} \mathrm{e}^{\mathrm{i}\omega g(b)}$ and $\frac{p(a)}{g'(a)} \mathrm{e}^{\mathrm{i}\omega g(a)}$ exist for all $p \in \mathcal{K}_n[\mathcal{M}, f]$, where if a or b is infinite they are defined by a limit. This condition is always true if a and b are both finite. When we use $\langle\!\langle \cdot, \cdot \rangle\!\rangle_m$ as our semi-inner product, we denote $v_n^{\mathcal{M}}$ and $Q_n^{\mathcal{M}}[f]$ as $v_{m,n}^{\mathcal{M}}$ and $Q_{m,n}^{\mathcal{M}}[f]$, respectively.

In addition to the properties of $Q_n^{\mathcal{M}}[f]$ already mentioned, we will prove the following facts:

(1) If $\langle \cdot, \cdot \rangle$ is an inner product and Arnoldi iteration fails, then $I[f] = Q_n^{\mathcal{M}}[f]$ except at finitely many choices of ω;

(2) If Arnoldi iteration succeeds, then

$$I[f] - Q_n^{\mathcal{M}}[f] = \mathcal{O}\Big(\omega^{-n-1}\Big)\,, \qquad \omega \to \infty;$$

(3) If Arnoldi iteration fails after r steps, then

$$I[f] - Q^{\mathcal{M}}_{m,n}[f] = \mathcal{O}\Big(\omega^{-r-2}\Big), \qquad \omega \to \infty.$$

Though a theory for Krylov subspace methods applied to bounded operators has been developed [**9**], it does not apply to unbounded, differential operators. Thus developing a theory for first order differential operators seems interesting in its own right. GMRES applied to the simplest such operator, the differentiation operator, was analyzed in [**13**], and this paper is a continuation of that one. Some other recent advances in applying matrix algorithms to functions include [**14**], which adapts Householder triangularization to orthogonalize a quasimatrix (i.e., a row vector whose columns are functions). Though in this paper we differentiate functions symbolically, a more numerical approach would be to utilize the `chebfun` system [**2**], which represents functions as Chebyshev polynomials of adaptive order. Indeed, the GMRES algorithm is built into `chebfun`, which makes implementation of $Q^{\mathcal{M}}_n[f]$ trivial.

In Section 2, we explain the details of the differential GMRES algorithm. In fact, a simple modification will allow us to reuse the Arnoldi process to compute $Q^{\mathcal{M}}_n[f]$ for additional values of ω; hence we only need to solve a finite-dimensional least squares problem with an Hessenberg matrix for each ω. Furthermore, we show that all condition numbers of this least squares problem converge to one as $\omega \to \infty$. We define a class of functions in Section 3 such that differential GMRES converges. Then, in Section 4, we prove the asymptotic properties of the method. Finally, we present some additional numerical results in Section 5. Here, we consider the case where f itself oscillates and we compute the Airy function along the negative real axis.

2. Algorithm

To simplify notation and reusability, we present many of the results in a general framework, replacing $C^\infty[\Omega]$ by a general vector space V with semi-inner product $\langle \cdot, \cdot \rangle$, and $\mathcal{L} : V \to V$ is a linear operator. We then use $\mathcal{M}_\omega$ to denote an operator of the form $\mathcal{P} + \mathrm{i}\omega$, where $\mathcal{P} : V \to V$ is a linear operator independent of ω. In our case $\mathcal{L}$, $\mathcal{M}$ and $\mathcal{P}$ are differential operators, hence they are not bounded, thus we use the following, weaker definition for boundedness:

Definition 2.1 For a linear operator $\mathcal{L} : V \to V$ and seminorm $\|\cdot\|$ on V, $\mathcal{B}_n[\mathcal{L}, \|\cdot\|]$ is the set of $f \in V$ such that $\|f\|, \|\mathcal{L}f\|, \left\|\mathcal{L}^2 f\right\|, \ldots, \left\|\mathcal{L}^{n-1} f\right\| < \infty$. We write $\mathcal{B}_n[\mathcal{L}]$ when the seminorm is implied by context.

This set satisfies the following properties:

- $\mathcal{B}_n[\mathcal{L}, \|\cdot\|]$ is a subspace of V;
- If $\mathcal{L}$ is bounded, then $\mathcal{B}_n[\mathcal{L}] = V$ for all n;
- For a second seminorm $|||\cdot|||$, $\mathcal{B}_n[\mathcal{L}, \|\cdot\| + |||\cdot|||] = \mathcal{B}_n[\mathcal{L}, \|\cdot\|] \cap \mathcal{B}_n[\mathcal{L}, |||\cdot|||]$;
- For a second linear operator $\mathcal{P} : V \to V$, $\mathcal{B}_n[\mathcal{L} + \mathcal{P}, \|\cdot\|] = \mathcal{B}_n[\mathcal{L}, \|\cdot\|] \cap \mathcal{B}_n[\mathcal{P}, \|\cdot\|]$;
- If Ω is a bounded interval and $\|\cdot\|$ is either $\|\cdot\|_1$, $\|\cdot\|_2$, $\|\cdot\|_\infty$ or $|||\cdot|||_m$, then, for any $\mathcal{L} : \mathbb{C}^\infty[a, b] \to \mathbb{C}^\infty[a, b]$, $\mathcal{B}_n[\mathcal{L}, \|\cdot\|] = \mathbb{C}^\infty[a, b]$ for all n.

The algorithm for computing $v_n^{\mathcal{L}}$ developed in [**13**] is virtually the same as the finite dimensional version of GMRES, the only difference being that a continuous semi-inner product $\langle\cdot,\cdot\rangle$ is used in place of the vector dot product. This algorithm depends on Arnoldi iteration, which determines a quasimatrix (or a row vector whose entries are elements of V) $\boldsymbol{q}_{n+1} = (q_1, \ldots, q_{n+1})$ whose columns are orthonormal, and an $(n + 1) \times n$ Hessenberg matrix H_n such that

$$\mathcal{L}\boldsymbol{q}_n = \boldsymbol{q}_{n+1} H_n.$$

We define the algorithm recursively as follows. (In practice, we can save memory by using only one function u for each $u_{i,j}$, though we write the subscripts explicitly as they will be used in the proofs below.)

Algorithm 2.2 *Arnoldi iteration*

Given $f \in \mathcal{B}_{n+1}[\mathcal{L}]$, compute $\boldsymbol{q}_{n+1}$ and H_n as follows:

1: *If $\|f\| = 0$, then set $\boldsymbol{q}_{n+1}$ and H_n both identically zero and return; otherwise,*

2: $q_1 = \frac{f}{\|f\|}$;

3: *For $k = 1, 2, \ldots, n$:*

  1: $u_{1,k} = \mathcal{L}q_k$;

  2: *For $j = 1, \ldots, k$: $h_{j,k} = \left\langle u_{j,k}, q_j \right\rangle$ and $u_{j+1,k} = u_{j,k} - h_{j,k} q_j$;*

  3: $h_{k+1,k} = \left\| u_{k+1,k1} \right\|$;

  4: *If $h_{k+1,k} \neq 0$ then $q_{k+1} = \frac{u_{k+1,k}}{h_{k+1,k}}$, otherwise we say that Arnoldi iteration failed at step k and set $q_{k+1} = 0$;*

4: *Return $\boldsymbol{q}_{n+1} = (q_1, \ldots, q_{n+1})$ and*

$$H_n = \begin{pmatrix} h_{1,1} & \cdots & h_{1,n} \\ h_{2,1} & \cdots & h_{2,n} \\ & \ddots & \vdots \\ & & h_{n+1,n} \end{pmatrix}.$$

The GMRES algorithm is now straightforward:

Algorithm 2.3 *GMRES*

Given $f \in \mathcal{B}_{n+1}[\mathcal{L}]$, compute $v_n^{\mathcal{L}}$ as follows:

1: *Find $\boldsymbol{q}_n$ and H_n using Arnoldi iteration (we do not need q_{n+1});*

2: *Use least squares to find coefficients $\boldsymbol{c} = (c_1, \ldots, c_n)^\top$ which minimize the norm*

$$\|H_n \boldsymbol{c} - \|f\| \boldsymbol{e}_1\|_2 ;$$

3: *Define*

$$v_n^{\mathcal{L}} = \boldsymbol{q}_n \boldsymbol{c} = \sum_{k=1}^{n} c_k q_k .$$

When $\langle \cdot, \cdot \rangle$ is an inner product or Arnoldi iteration succeeds, the columns of $\boldsymbol{q}_n$ span $\mathcal{K}_n[\mathcal{L}, f]$. Thus GMRES does indeed compute an element with minimal seminorm:

$$\|\mathcal{L}\boldsymbol{q}_n \boldsymbol{c} - f\| = \|\boldsymbol{q}_{n+1} H_n \boldsymbol{c} - \|f\| \boldsymbol{q}_1\| = \|\boldsymbol{q}_{n+1} \left[H_n \boldsymbol{c} - \|f\| \boldsymbol{e}_1\right]\| = \|H_n \boldsymbol{c} - \|f\| \boldsymbol{e}_1\| .$$

When we apply Arnoldi iteration to the operator $\mathcal{M}$, we denote the Hessenberg matrix returned by $H_{n,\omega}$, to emphasize the dependence on ω. If we used this algorithm without modification, we would have to recompute the approximation from scratch for each choice of ω. But, due to the special structure of our operator, we can actually reuse most of the computation for other choices of ω. The key is the following theorem:

Theorem 2.4 *Suppose $f \in \mathcal{B}_{n+1}[\mathcal{P}]$ and that Arnoldi iteration with $\mathcal{P}$ and f succeeds, returning $\tilde{\boldsymbol{q}}_n$ and $\tilde{H}_n$. Then Arnoldi iteration applied to the operator $\mathcal{M} = \mathcal{P} + \mathrm{i}\omega$ returns $\boldsymbol{q}_n = \tilde{\boldsymbol{q}}_n$ and the Hessenberg matrix*

$$H_{n,\omega} = \tilde{H}_n + \mathrm{i}\omega I_{n+1,n} \qquad \text{for the } n+1 \times n \text{ matrix} \qquad I_{n+1,n} = \begin{pmatrix} 1 & & \\ & \ddots & \\ & & 1 \\ & & \end{pmatrix} .$$

Proof: We first show that $\boldsymbol{q}_n = \tilde{\boldsymbol{q}}_n$. The theorem is trivially true for $q_1 = \frac{f}{\|f\|}$. Now assume that $\boldsymbol{q}_k = \tilde{\boldsymbol{q}}_k$ Note that

$$q_{k+1} \in \operatorname{span}\{q_1, \ldots, q_k, \mathcal{P}q_k + \mathrm{i}\omega q_k\} = \operatorname{span}\{q_1, \ldots, q_k, \mathcal{P}q_k\} . \tag{2.1}$$

The element in the space $\operatorname{span}\{q_1, \ldots, q_k, \mathcal{P}q_k\}$ orthonormal to $\boldsymbol{q}_k$ is unique, hence $\boldsymbol{q}_{k+1}$ must be equal $\tilde{\boldsymbol{q}}_{k+1}$.

Now let $\tilde{h}_{i,j}$ be the (i, j)th entry of the matrix $\tilde{H}_n$. Then, for $i \leq j + 1$,

$$h_{i,j} = \langle \boldsymbol{q}_{n+1} H_{n,\omega} \boldsymbol{e}_i, q_j \rangle = \langle (\mathcal{P} + \mathrm{i}\omega) \boldsymbol{q}_n \boldsymbol{e}_i, q_j \rangle$$

$$= \langle \mathcal{P} q_i, q_j \rangle + \mathrm{i}\omega \langle q_i, q_j \rangle = \left\langle \boldsymbol{q}_{n+1} \tilde{H}_n \boldsymbol{e}_i, q_j \right\rangle + \mathrm{i}\omega\delta_{i,j} = \tilde{h}_{i,j} + \mathrm{i}\omega\delta_{i,j}.$$

Q.E.D.

We use this theorem to alter the GMRES algorithm:

Algorithm 2.5 *Modified GMRES*

Given $f \in \mathcal{B}_{n+1}[\mathcal{P}]$, compute $v_n^{\mathcal{M}}$ as follows:

1: *Precompute $\boldsymbol{q}_n$ and $\tilde{H}_n$ using Arnoldi iteration with $\mathcal{P}$ and f;*

2: *Define $H_{n,\omega} = \tilde{H}_n + \mathrm{i}\omega I_{n+1,n}$;*

3: *Use least squares to find coefficients $\boldsymbol{c} = (c_1, \ldots, c_n)^\top$ which minimize the norm*

$$\left\| H_{n,\omega}\boldsymbol{c} - \|f\| \, \boldsymbol{e}_1 \right\|_2 ;$$

4: *Define*

$$v_n^{\mathcal{M}} = \boldsymbol{q}_n \boldsymbol{c} = \sum_{k=1}^{n} c_k q_k.$$

We can use this formulation to say something about the stability of the algorithm. We will show that the least squares step is well-conditioned as $\omega \to \infty$. This is confirmed in numerical experiments, where larger ω results in better numerical stability.

Corollary 2.6 *For any condition number κ and fixed n, $\kappa(H_{n,\omega}) \to 1$ as $\omega \to \infty$.*

Proof:

Note that

$$H_{n,\omega}^{\star} H_{n,\omega} = H_{n,0}{}^{\star} H_{n,0} + \mathrm{i}\omega (H_{n,0}{}^{\star} I_{n+1,n} + I_{n+1,n} H_{n,0}) - \omega^2 I_n.$$

Since the condition number κ of a nonsingular matrix depends continuously on its entries, we obtain

$$\kappa(H_{n,\omega}^{\star} H_{n,\omega}) = \kappa\Big(\omega^2 \left[I_n + \mathcal{O}\big(\omega^{-1}\big) \right]\Big) = \kappa\Big(I_n + \mathcal{O}\big(\omega^{-1}\big)\Big) \to \kappa(I_n) = 1.$$

Q.E.D.

3. Convergence

As with any numerical method, an important question is whether the computed results converge to the true solution. In this section we will derive fairly weak conditions on f and g which ensure convergence. As an example, consider the integral

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

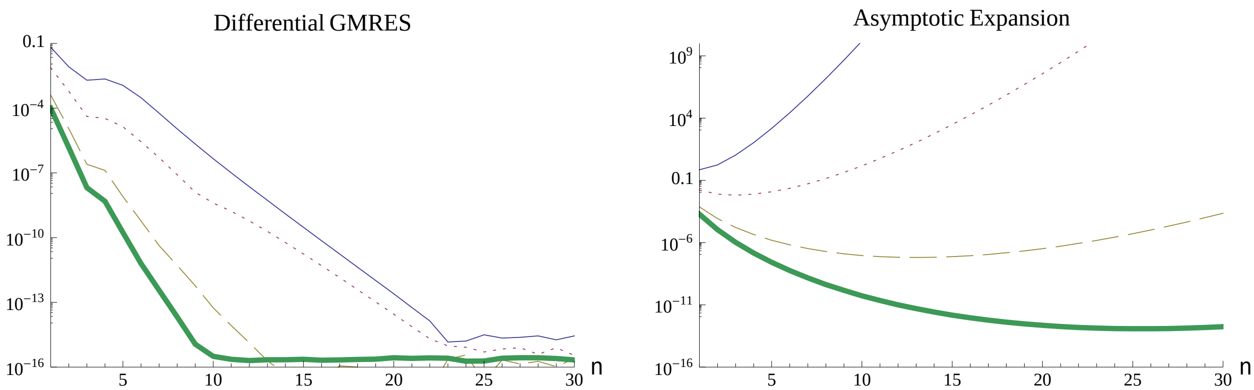

Figure 1: Errors in approximating $\int_0^1 \cos x \, \mathrm{e}^{\mathrm{i}\omega(x^2+x)} \, \mathrm{d}x$ by $Q_n^{\mathcal{M}}[f]$ (left) and the n-term asymptotic expansion (right) for $\omega = 1$ (plain), 10 (dotted), 50 (dashed) and 100 (thick).

In Figure 1 we compare the error in approximating $I[f]$ (computed by Mathematica using the `NIntegrate` routine) by $Q_n^{\mathcal{M}}[f]$ to that of the asymptotic expansion of the same order, for $\omega = 1, 10, 50$ and 100. As can be seen, this new method converge for each choice of ω, while the asymptotic expansion diverges super-geometrically fast.

Recall that $\|\cdot\|_S$ denote the supremum norm over a set S of complex points. Now define the following class of functions:

Definition 3.1 $\mathcal{G}[\mathcal{L}, \Omega]$ is the class of functions $f \in \mathbb{C}^\infty[\Omega]$ such that for every $\epsilon > 0$ there exists an n and a $g \in \mathcal{K}_n[\mathcal{L}, f]$ such that

$$\|f - \mathcal{L}g\|_\Omega < \epsilon.$$

When Ω is bounded, convergence in the supremum norm immediately implies convergence in the L_2 norm. Thus, if $f \in \mathcal{G}[\mathcal{M}, \Omega]$, then

$$\left| I[f] - Q_n^{\mathcal{M}}[f] \right| = \left| I\left[f - \mathcal{M} v_n^{\mathcal{M}}\right] \right| \leq \sqrt{b-a} \left\| f - \mathcal{M} v_n^{\mathcal{M}} \right\|_2 \to 0, \qquad \text{as } n \to \infty.$$

Since g is monotonic and smooth, its inverse exists and is $\mathbb{C}^\infty[\mathrm{cl}\,(g(a), g(b))]$. Consider the function

$$w(t) = \frac{f(g^{-1}(t))}{g'(g^{-1}(t))} \mathrm{e}^{\mathrm{i}\omega t}, \qquad \text{for } t \in \mathrm{cl}\,(g(a), g(b)).$$

Note that

$$w'(t) = \left[\frac{f'(g^{-1}(t))}{g'(g^{-1}(t))^2} - \frac{f(g^{-1}(t)) g''(g^{-1}(t))}{g'(g^{-1}(t))^3} + \mathrm{i}\omega \frac{f(g^{-1}(t))}{g'(g^{-1}(t))} \right] \mathrm{e}^{\mathrm{i}\omega t} = \frac{\mathcal{M} f(g^{-1}(t))}{g'(g^{-1}(t))} \mathrm{e}^{\mathrm{i}\omega t}.$$

Induction reveals that

$$w^{(k)}(t) = \frac{\mathcal{M}^k f(g^{-1}(t))}{g'(g^{-1}(t))} \mathrm{e}^{\mathrm{i}\omega t},$$

and hence

$$g'(x)\mathrm{e}^{-\mathrm{i}\omega g(x)}\mathrm{span}\left\{w(g(x)),\ldots,w^{(n-1)}(g(x))\right\} = \mathcal{K}_n[\mathcal{M},f]\,.$$

Thus $f \in \mathcal{G}[\mathcal{M},\Omega]$ if and only if $w \in \mathcal{G}[\mathcal{D},\mathrm{cl}\,(g(a),g(b))]$.

Conditions for which a function can be approximated by its own derivatives in Ω were derived in [**13**]. These conditions require the following class:

Definition 3.2 For a sequence of open balls $\boldsymbol{B} = \{B_1, B_2, \ldots\}$ in the complex plane (i.e., $B_k = \{z : |z - p_k| < \epsilon_k\}$ for some complex point p_k and positive real number ϵ_k), $\mathcal{P}[\Omega, \boldsymbol{B}]$ is the set of functions f defined for every ball in $\boldsymbol{B}$ such that $\|f\|_{\Omega+B_k} \to 0$ as $k \to \infty$.

Definition 3.3 $\mathcal{P}[\Omega]$ is the union of $\mathcal{P}[\Omega, \boldsymbol{B}]$ over all sequences $\boldsymbol{B}$.

The following theorem states that a function which decays in the complex plane in a sequence of domains larger than Ω can be approximated by its derivatives in Ω, subject to some minor conditions on analyticity.

Theorem 3.4 [**13**] *$w \in \mathcal{G}[\mathcal{D},\Omega]$ if either of the following conditions hold:*

- *w is entire, Ω is bounded and $w \in \mathcal{P}[\Omega]$;*
- *w is analytic in a domain D, $w \in \mathcal{P}[\Omega, \boldsymbol{B}]$ where zero and $\boldsymbol{B}$ are in an open simply connected domain U such that $U + \Omega \subset D$, and w is bounded in $u + \Omega$ for all $u \in U$.*

The presence of the $\mathrm{e}^{\mathrm{i}\omega t}$ kernel in w allows us to find a simpler (but weaker) condition that ensures convergence:

Corollary 3.5 *Suppose that $f(g^{-1}(t))/g'(g^{-1}(t))$ can be analytically continued to a function which has finitely many singularities and at most exponential growth in the first quadrant of the complex plane, and that a is bounded. Then $f \in \mathcal{G}[\mathcal{M},\Omega]$ for sufficiently large ω.*

In analogy to the finite dimensional case, linear dependence of $f, \mathcal{M}f, \ldots, \mathcal{M}^{n-1}f$ typically implies convergence of GMRES:

Theorem 3.6 *If $\langle\cdot,\cdot\rangle$ is an inner product, $f \in \mathcal{B}_{n+1}[\mathcal{L}]$ and the dimension of $\mathcal{K}_n[\mathcal{M}, f]$ is $r < n$ for some $n \geq 1$, then $Q_n^{\mathcal{M}}[f] = I[f]$ except for at most r values of ω.*

Proof: Arnoldi iteration gives us a Hessenberg matrix $H_{r,\omega}$ such that $\mathcal{M}\boldsymbol{q}_r = \boldsymbol{q}_{r+1}H_{r,\omega}$, where $q_{r+1} = 0$. Define $\hat{H}_{r,\omega}$ as the square matrix consisting of the upper-left $r \times r$ block of $H_{r,\omega}$. Thus (note that the dimension of $\boldsymbol{e}_1$ changes)

$$\left\|\mathcal{M}v_n^{\mathcal{M}} - f\right\| = \left\|\boldsymbol{q}_{r+1}\left[H_{r,\omega}\boldsymbol{c} - \|f\|\,\boldsymbol{e}_1\right]\right\| = \left\|\boldsymbol{q}_r\left[\hat{H}_{r,\omega}\boldsymbol{c} - \|f\|\,\boldsymbol{e}_1\right]\right\| = \left\|\hat{H}_{r,\omega}\boldsymbol{c} - \|f\|\,\boldsymbol{e}_1\right\|_2.$$

We know that $\hat{H}_{r,\omega} = \hat{H}_{r,0} + \mathrm{i}\omega I_r$; hence $\det \hat{H}_{r,\omega}$ is a degree-r polynomial in ω. Since the inverse of a nonsingular matrix depends continuously on its entries, $\hat{H}_{r,\omega}$ is nonsingular for sufficiently large ω, which implies that $\det \hat{H}_{r,\omega}$ is not identically zero as a function of ω. Thus there are at most r values of ω such that $\det \hat{H}_{r,\omega}$ vanishes. When this determinant does not vanish, setting $\boldsymbol{c} = \hat{H}_{r,\omega}^{-1}\boldsymbol{e}_1$ results in $\left\| \mathcal{M} v_n^{\mathcal{M}} - f \right\| = 0$. Thus $f = \mathcal{M} v_n^{\mathcal{M}}$ (since both functions are continuous), and hence

$$I[f] = I\Big[\mathcal{M} v_n^{\mathcal{M}}\Big] = Q_n^{\mathcal{M}}[f]\,.$$

Q.E.D.

4. Asymptotics

As seen in Figure 1, not only does differential GMRES converge, but in fact the rate of convergence increases as the frequency increases. In this section we explain this phenomenon by proving that the error behaves like $\mathcal{O}\Big(\omega^{-n-1}\Big)$ as $\omega \to \infty$. Consider again the integral

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

Instead of investigating the behaviour of the error of $Q_n^{\mathcal{M}}[f]$ as $n \to \infty$ with fixed ω, we want to see how the error behaves as $\omega \to \infty$ with fixed n. In Figure 2 we compare the error in approximating $I[f]$ by $Q_n^{\mathcal{M}}[f]$ to that of the asymptotic expansion of the same order, for $n = 3$, 6, 10 and 20. Note that the peaks in the top-left graph are not singularities. While both the n-term asymptotic expansion and $Q_n^{\mathcal{M}}[f]$ decay at the same rate as $\omega \to \infty$, a dramatic increase in accuracy over the asymptotic expansion is obtained, with the increase becoming more significant as n increases.

To establish the asymptotic order of $Q_n^{\mathcal{M}}[f]$, we will show that it must take into account the behaviour of the asymptotic expansion. Thus we first present a derivation of the asymptotic expansion of a particular solution of $\mathcal{L}v = f$. An asymptotic expansion for the integral $I[f]$ is typically found using integration by parts. We, however, want a solution to the associated differential equation, and hence we use a slightly different, though equivalent, formulation. We will require the following lemmas in several of the proofs that follow. The first lemma states that any two seminorms are in some sense asymptotically equivalent for functions in $\mathcal{K}_n[\mathcal{M}, f]$.

Lemma 4.1 *Let $|||\cdot|||$ be a seminorm and $f \in \mathcal{B}_n\left[\mathcal{D}\frac{1}{g'}, \|\cdot\| + |||\cdot|||\right]$, and assume that $n-1$ Arnoldi iterations succeed, or that $\langle\cdot,\cdot\rangle$ is an inner product. If $p_\omega \in \mathcal{K}_n[\mathcal{M}, f]$ and $\|p_\omega\| = \mathcal{O}(1)$, as $\omega \to \infty$, then $|||\, p_\omega \,||| = \mathcal{O}(1)$.*

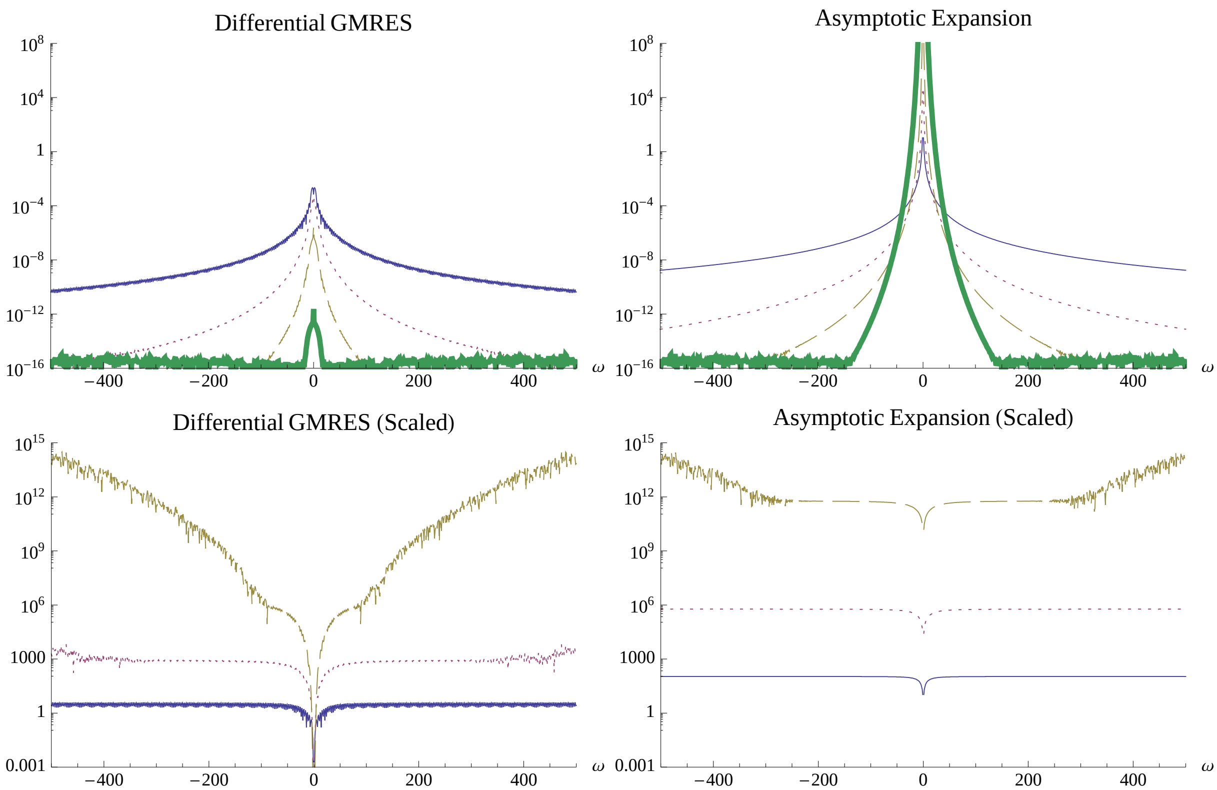

Figure 2: Errors in approximating $\int_0^1 \cos x\, \mathrm{e}^{\mathrm{i}\omega(x^2+x)}\, \mathrm{d}x$. In the top graphs, error for $Q_n^{\mathcal{M}}[f]$ (left) and the n-term asymptotic expansion (right), for $n = 3$ (plain) 6 (dotted), 10 (dashed) and 20 (thick). In the bottom graphs the same errors, each scaled by ω^{n+1}.

Proof: Suppose $\mathcal{K}_n[\mathcal{M}, f]$ has dimension r. Let $\boldsymbol{q}_r$ be the basis for $\mathcal{K}_n[\mathcal{M}, f]$ obtained via $r-1$ Arnoldi iterations with $\langle\cdot,\cdot\rangle$, which Theorem 2.4 states is independent of ω. Thus $p_\omega(x) = \boldsymbol{q}_r(x)\boldsymbol{c}_\omega$ where $\boldsymbol{c}_\omega$ is independent of x. Note that $\|\boldsymbol{c}_\omega\|_2 = \|p_\omega\| = \mathcal{O}(1)$. Then

$$|||\, p_\omega \,||| = |||\, \boldsymbol{q}_r \boldsymbol{c}_\omega \,||| \leq n \max\{|||\, q_1 \,|||, \ldots, |||\, q_r \,|||\} \, \|\boldsymbol{c}_\omega\|_\infty = \mathcal{O}(1)\,, \qquad \omega \to \infty.$$

Q.E.D.

Lemma 4.2 *Let* $f \in \mathcal{B}_m\left[\mathcal{D}\frac{1}{g'}, \|\cdot\| + \left\|\frac{\cdot}{g'}\right\|_\infty + \left\|\mathcal{D}\frac{1}{g'}\cdot\right\|_1\right]$, *and assume that* $m-1$ *Arnoldi iterations succeed, or that* $\langle\cdot,\cdot\rangle$ *is an inner product. Suppose we are given* $p_\omega \in \mathcal{K}_n[\mathcal{M}, f]$ *such that* $\|p_\omega\| = \mathcal{O}\left(\omega^{-s}\right)$. *If* $m \geq n$, *then*

$$I[p_\omega] = \mathcal{O}\left(\omega^{-s-1}\right).$$

Furthermore, if $m \geq n+1$ *and* $0 = \frac{p_\omega(a)}{g'(a)} = \frac{p_\omega(b)}{g'(b)}$, *then*

$$I[p_\omega] = \mathcal{O}\left(\omega^{-s-2}\right).$$

Proof:

Note that $\omega^s p_\omega$ satisfies the conditions of the preceding lemma with $|||\cdot||| = \left\|\mathcal{D}\frac{1}{g'}\cdot\right\|_1 + \left\|\frac{\cdot}{g'}\right\|_\infty$, hence $|||\, p_\omega \,||| = \mathcal{O}\left(\omega^{-s}\right)$. Integrating by parts we obtain

$$\begin{aligned}|I[p_\omega]| &= \left|\int_a^b \mathrm{e}^{\mathrm{i}\omega g} p_\omega \,\mathrm{d}x\right| = \left|\frac{1}{\mathrm{i}\omega}\left[\frac{p_\omega(b)}{g'(b)}\mathrm{e}^{\mathrm{i}\omega g(b)} - \frac{p_\omega(a)}{g'(a)}\mathrm{e}^{\mathrm{i}\omega g(a)}\right] - \frac{1}{\mathrm{i}\omega} I\left[\mathcal{D}\frac{p_\omega}{g'}\right]\right| \\ &\leq \frac{3}{\omega}|||\, p_\omega \,||| = \mathcal{O}\left(\omega^{-s-1}\right).\end{aligned}$$

(Recall that we have assumed that $\frac{p_\omega(b)}{g'(b)}\mathrm{e}^{\mathrm{i}\omega g(b)}$ and $\frac{p_\omega(a)}{g'(a)}\mathrm{e}^{\mathrm{i}\omega g(a)}$ exist.) For the second part of the theorem we note that the first term in the above expansion is zero, and by integrating by parts once more we obtain:

$$\begin{aligned}I[p_\omega] &= -\frac{1}{\mathrm{i}\omega} I\left[\mathcal{D}\frac{p_\omega}{g'}\right] \\ &= \frac{1}{\omega^2}\left\{\frac{1}{g'(b)}\mathcal{D}\left[\frac{p_\omega}{g'}\right](b)\mathrm{e}^{\mathrm{i}\omega g(b)} - \frac{1}{g'(a)}\mathcal{D}\left[\frac{p_\omega}{g'}\right](a)\mathrm{e}^{\mathrm{i}\omega g(a)}\right\} - \frac{1}{\omega^2} I\left[\left(\mathcal{D}\frac{1}{g'}\right)^2 p_\omega\right] \\ &= \mathcal{O}\left(\omega^{-s-2}\right).\end{aligned}$$

Q.E.D.

We now obtain the classical asymptotic expansion:

Theorem 4.3 *Let* $f \in \mathcal{B}_{n+1}\left[\mathcal{D}\frac{1}{g'}, \|\cdot\| + \left\|\frac{\cdot}{g'}\right\|_\infty + \left\|\mathcal{D}\frac{1}{g'}\cdot\right\|_1\right]$, *and assume that* n *Arnoldi iterations succeed, or that* $\langle\cdot,\cdot\rangle$ *is an inner product. The residual of the asymptotic expansion is*

$$\left\|f - \mathcal{L}v_n^{\mathrm{A}}\right\| = \mathcal{O}\left(\omega^{-n}\right) \qquad \text{for} \qquad v_n^{\mathrm{A}} = -\sum_{k=1}^{n}(-\mathrm{i}\omega)^{-k}\frac{1}{g'}\left(\mathcal{D}\frac{1}{g'}\right)^{k-1} f.$$

Furthermore

$$I[f] - Q_n^{\mathrm{A}}[f] = \mathcal{O}\left(\omega^{-n-1}\right),$$

where

$$Q_n^{\mathrm{A}}[f] = I\left[\mathcal{L}v_n^{\mathrm{A}}\right] = v_n^{\mathrm{A}}(b)\mathrm{e}^{\mathrm{i}\omega g(b)} - v_n^{\mathrm{A}}(a)\mathrm{e}^{\mathrm{i}\omega g(a)}.$$

Proof: Clearly

$$\left\|f - \mathcal{L}v_1^{\mathrm{A}}\right\| = \left\|\mathcal{D}v_1^{\mathrm{A}}\right\| = \frac{1}{\mathrm{i}\omega}\left\|\mathcal{D}\frac{1}{g'}f\right\| = \mathcal{O}\left(\omega^{-1}\right).$$

The first part of the theorem then follows from induction. From (2.1) we know that

$$\mathcal{K}_n[\mathcal{M}, f] = \operatorname{span}\left\{ f, \mathcal{D}\frac{1}{g'}f, \left(\mathcal{D}\frac{1}{g'}\right)^2 f, \ldots, \left(\mathcal{D}\frac{1}{g'}\right)^{n-1} f \right\} = \mathcal{K}_n\left[\mathcal{D}\frac{1}{g'}, f\right].$$

It follows that $g' v_n^{\mathrm{A}} \in \mathcal{K}_n[\mathcal{M}, f]$. The theorem follows from Lemma 4.2 with

$$p_\omega = f - \mathcal{L}v_n^{\mathrm{A}} = f - \mathcal{M}g' v_n^{\mathrm{A}} \in \mathcal{K}_{n+1}[\mathcal{M}, f].$$

Q.E.D.

The residual of the differential GMRES approximation must be smaller than that of the asymptotic expansion:

Lemma 4.4 *Let* $f \in \mathcal{B}_{n+1}\left[\mathcal{D}\frac{1}{g'}, \|\cdot\| + \left\|\frac{\cdot}{g'}\right\|_\infty + \left\|\mathcal{D}\frac{1}{g'}\cdot\right\|_1\right]$, *and assume that n Arnoldi iterations succeed, or that $\langle\cdot,\cdot\rangle$ is an inner product. Then*

$$\left\| f - \mathcal{M}v_n^{\mathcal{M}} \right\| = \mathcal{O}\left(\omega^{-n}\right).$$

Proof: Since GMRES minimizes the seminorm the residual, $\mathcal{M}v_n^{\mathcal{M}}$ must approximate f better than the asymptotic expansion:

$$\left\| f - \mathcal{M}v_n^{\mathcal{M}} \right\| \le \left\| f - \mathcal{M}g' v_n^{\mathrm{A}} \right\| = \left\| f - \mathcal{L}v_n^{\mathrm{A}} \right\| = \mathcal{O}\left(\omega^{-n}\right).$$

Q.E.D.

When Ω is bounded, a bound on the residual automatically gives us a bound on the quadrature error:

$$\left| I[f] - Q_n^{\mathcal{M}}[f] \right| = \left| I\left[f - \mathcal{M}v_n^{\mathcal{M}} \right] \right| \le \sqrt{b-a} \left\| f - \mathcal{M}v_n^{\mathcal{M}} \right\|_2 = \mathcal{O}\left(\omega^{-n}\right).$$

However, this bound is not sharp: we actually achieve an order of accuracy of $\mathcal{O}\left(\omega^{-n-1}\right)$.

Theorem 4.5 *Let* $f \in \mathcal{B}_{n+1}\left[\mathcal{D}\frac{1}{g'}, \|\cdot\| + \left\|\frac{\cdot}{g'}\right\|_\infty + \left\|\mathcal{D}\frac{1}{g'}\cdot\right\|_1\right]$, *and assume that n Arnoldi iterations succeed, or that $\langle\cdot,\cdot\rangle$ is an inner product. Then*

$$Q_n^{\mathcal{M}}[f] - I[f] = \mathcal{O}\left(\omega^{-n-1}\right).$$

Proof: This estimate follows by combining the fact that $f - \mathcal{M}v_n^{\mathcal{M}} \in \mathcal{K}_{n+1}[\mathcal{M}, f]$ with Lemma 4.4 and Lemma 4.2.

Q.E.D.

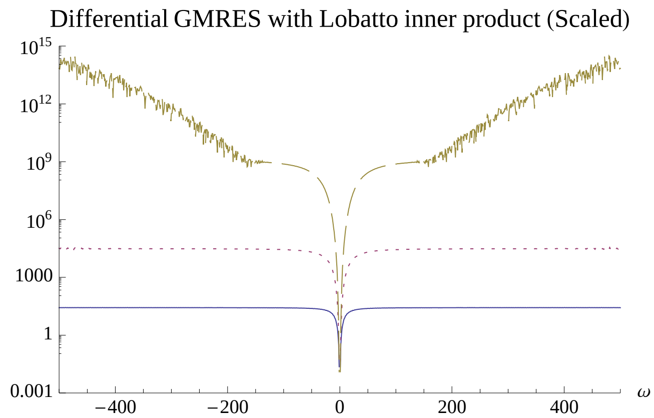

Figure 3: The error scaled by ω^{n+2} in approximating $\int_0^1 \cos x\, \mathrm{e}^{\mathrm{i}\omega(x^2+x)}\, \mathrm{d}x$ by $Q_{n,n}^{\mathcal{M}}$ for $n = 2$ (plain) 5 (dotted) and 9 (dashed).

Though the integrals we are computing are oscillatory, the elements of the Krylov subspace are not, at least with respect to $\omega \to \infty$. However, the higher order elements of the orthogonal basis $\{q_1, \ldots, q_n\}$ are typically oscillatory with respect to $n \to \infty$, which means that computing L_2 inner products in the Arnoldi process becomes increasingly difficult as $n \to \infty$. To avoid this issue, we replace the continuous inner product with the discretization $\langle\!\langle \cdot, \cdot \rangle\!\rangle_m$, based on Clenshaw–Curtis quadrature with m points. This raises the question: is the asymptotic accuracy maintained? The answer to the question is largely affirmative, though it depends on how many iterations of Arnoldi can successfully be performed. We actually get a higher asymptotic order with the discrete semi-inner product if $m = n$ and Arnoldi fails at the nth iteration. This is seen in Figure 3, where the same asymptotic orders as in Figure 2 are achieved with one less iteration. In this case, $\mathcal{M} v_{m,n}^{\mathcal{M}}$ actually interpolates f at the quadrature points, and hence preconditioned differential GMRES is essentially a numerically stable way of computing a Levin-type method with the asymptotic basis, developed in [**10**].

Theorem 4.6 *Suppose that* $f \in \mathcal{B}_{n+1}\left[\mathcal{D}\frac{1}{g'}, \|\cdot\| + |\!|\!| \cdot |\!|\!| + \left\|\frac{\cdot}{g'}\right\|_\infty + \left\|\mathcal{D}\frac{1}{g'}\cdot\right\|_1\right]$, *where* $\langle \cdot, \cdot \rangle$ *is an inner product and* $\langle\!\langle \cdot, \cdot \rangle\!\rangle$ *is a semi-inner product such that* $|\!|\!| p |\!|\!| = 0$ *implies that* $\frac{p(a)}{g'(a)} = \frac{p(b)}{g'(b)} = 0$ *for all* $p \in \mathcal{K}_n[\mathcal{M}, f]$. *If Arnoldi iteration with* $\langle\!\langle \cdot, \cdot \rangle\!\rangle$ *fails at* r *iterations, then*

$$I[f] - Q_{m,n}^{\mathcal{M}}[f] = \mathcal{O}\left(\omega^{-r-2}\right), \qquad \omega \to \infty.$$

Otherwise,

$$I[f] - Q_{m,n}^{\mathcal{M}}[f] = \mathcal{O}\left(\omega^{-n-1}\right), \qquad \omega \to \infty.$$

Proof:

When Arnoldi iteration succeeds, the theorem follows from Theorem 4.5. Otherwise, we have $\mathcal{M}\boldsymbol{q}_r = \boldsymbol{q}_{r+1}H_{r,\omega} + u_{r+1,r}\boldsymbol{e}_r^\top$, where $q_{r+1} = 0$ and $|||\, u_{r+1,r} \,||| = 0$. Using the notation of the proof of Theorem 2.4, we find that $u_{r+1,r}$ is independent of ω:

$$u_{r+1,r} = \mathcal{M}q_r - \sum_{j=1}^{r} h_{j,r}q_j = \mathcal{D}\frac{q_r}{g'} + \mathrm{i}\omega q_r - \sum_{j=1}^{r} \tilde{h}_{j,r}q_j - \mathrm{i}\omega q_r = \mathcal{D}\frac{q_r}{g'} - \sum_{j=1}^{r} \tilde{h}_{j,r}q_j.$$

Similar to the proof of Theorem 3.6,

$$|||\, \mathcal{M}v_{m,n}^{\mathcal{M}} - f \,||| = |||\, \boldsymbol{q}_{r+1}\left[H_{r,\omega}\boldsymbol{c} - |||\, f \,|||\boldsymbol{e}_1\right] \,||| = \left\|\hat{H}_{r,\omega}\boldsymbol{c} - |||\, f \,|||\boldsymbol{e}_1\right\|_2. \tag{4.1}$$

Again, large ω ensures that $\hat{H}_{r,\omega}$ is nonsingular; thence, $\hat{H}_{r,\omega}\boldsymbol{c} - |||\, f \,|||\boldsymbol{e}_1 = 0$. Thus

$$\left\|\mathcal{M}v_{m,n}^{\mathcal{M}} - f\right\| = \left\|\boldsymbol{q}_r\left[\hat{H}_{r,\omega}\boldsymbol{c} - |||\, f \,|||\boldsymbol{e}_1\right] + c_r u_{r+1,r}\right\| = |c_r|\,\|u_{r+1,r}\|\,.$$

We need to find the asymptotic order of c_r. Note that, for sufficiently large ω,

$$\begin{aligned}\boldsymbol{c} &= |||\, f \,|||\hat{H}_{r,\omega}^{-1}\boldsymbol{e}_1 = \frac{1}{\mathrm{i}\omega}|||\, f \,|||\left(\frac{1}{\mathrm{i}\omega}\hat{H}_{r,0} + I_r\right)^{-1}\boldsymbol{e}_1 \\ &= \frac{1}{\mathrm{i}\omega}|||\, f \,|||\left[I_r - \frac{1}{\mathrm{i}\omega}\hat{H}_{r,0} + \left(-\frac{1}{\mathrm{i}\omega}\hat{H}_{r,0}\right)^2 + \cdots + \left(-\frac{1}{\mathrm{i}\omega}\hat{H}_{r,0}\right)^{r-1} + \mathcal{O}\left(\omega^{-r}\right)\right]\boldsymbol{e}_1.\end{aligned}$$

Since $\hat{H}_{r,0}$ is Hessenberg, the last row of $\hat{H}_{r,0}^k\boldsymbol{e}_1$ is zero for $k \leq r-2$. Thus $c_r = \mathcal{O}\left(\omega^{-r}\right)$, and $\left\|\mathcal{M}v_{m,n}^{\mathcal{M}} - f\right\| = \mathcal{O}\left(\omega^{-r}\right)$. We can apply the second part of Lemma 4.2 with $p_\omega = \mathcal{M}v_{m,n}^{\mathcal{M}} - f$; hence,

$$I[f] - Q_{m,n}^{\mathcal{M}}[f] = I\left[f - \mathcal{M}v_{m,n}^{\mathcal{M}}\right] = \mathcal{O}\left(\omega^{-r-2}\right).$$

Q.E.D.

5. Numerical results

In most of the following examples, Ω is bounded, so the conditions on f being in $\mathcal{B}_{n+1}[\mathcal{M}]$ are satisfied for all the norms considered. One property of the differential GMRES method we have not yet explored is that it does not depend on ω being real. In Figure 4 we compute

$$I[1] = \int_0^1 \mathrm{e}^{\mathrm{i}\omega \sin x}\,\mathrm{d}x$$

for ω on four circles in the complex plane. As can be seen, differential GMRES in some sense approximates the integral uniformly throughout the complex plane. Note that the relative error will still explode at zeros of $I[1]$, and thus a more sensible "relative error" would be

$$\frac{\left|I[1] - Q_n^{\mathcal{M}}[1]\right|}{\left\|\mathrm{e}^{\mathrm{i}\omega g}\right\|_2},$$

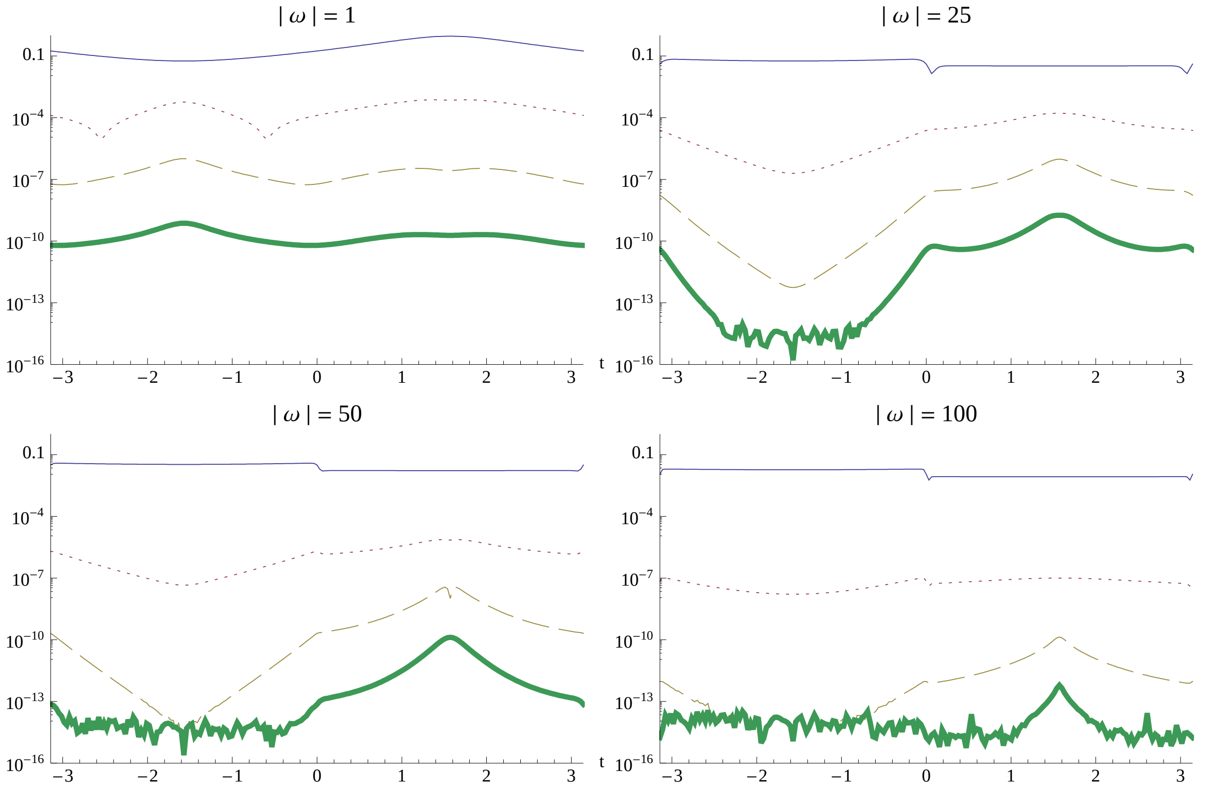

Figure 4: The relative error in approximating $\int_0^1 \mathrm{e}^{\mathrm{i}\omega \sin x}\,\mathrm{d}x$ by $Q_n^{\mathcal{M}}[f]$ for $n = 1$ (plain), 5 (dotted), 10 (dashed) and 15 (thick) and $\omega = \mathrm{e}^{\mathrm{i}t}$, $25\mathrm{e}^{\mathrm{i}t}$, $50\mathrm{e}^{\mathrm{i}t}$ and $100\mathrm{e}^{\mathrm{i}t}$.

in which case uniform convergence follows from the bound

$$\left|I[1] - Q_n^{\mathcal{M}}[1]\right| = \left|I\left[1 - \mathcal{M}v_n^{\mathcal{M}}\right]\right| \leq \left\|1 - \mathcal{M}v_n^{\mathcal{M}}\right\|_2 \left\|\mathrm{e}^{\mathrm{i}\omega g}\right\|_2.$$

Remark: To compute the exact values of the integral, we had to increase the working precision of MATHEMATICA's `NIntegrate` to 20 digits. Computing $Q_n^{\mathcal{M}}[1]$ still only used machine precision arithmetic.

A class of integrals where differential GMRES significantly outperforms other oscillatory methods are those in which f itself has oscillations in the form of an exponential oscillator. Filon-type, moment-free Filon-type and Levin-type methods are all based on polynomial approximation, which cannot capture oscillations in f without using high degree polynomials. Suppose that $f = r\mathrm{e}^{\mathrm{i}kp}$ where $p' \neq 0$, r and p are smooth functions and k is real. Note that

$$\mathcal{M}f = \mathrm{e}^{\mathrm{i}kp}\left[\mathcal{D}\frac{1}{g'} + \mathrm{i}k\frac{p'}{g'} + \mathrm{i}\omega\right] r.$$

It follows that applying $\mathcal{M}$ to f results in a function with the same kernel of oscillations, hence we can write any function in $\mathcal{K}_n[\mathcal{M}, f]$ as $\tilde{r}\mathrm{e}^{\mathrm{i}kp}$ for some nonoscillatory (with respect

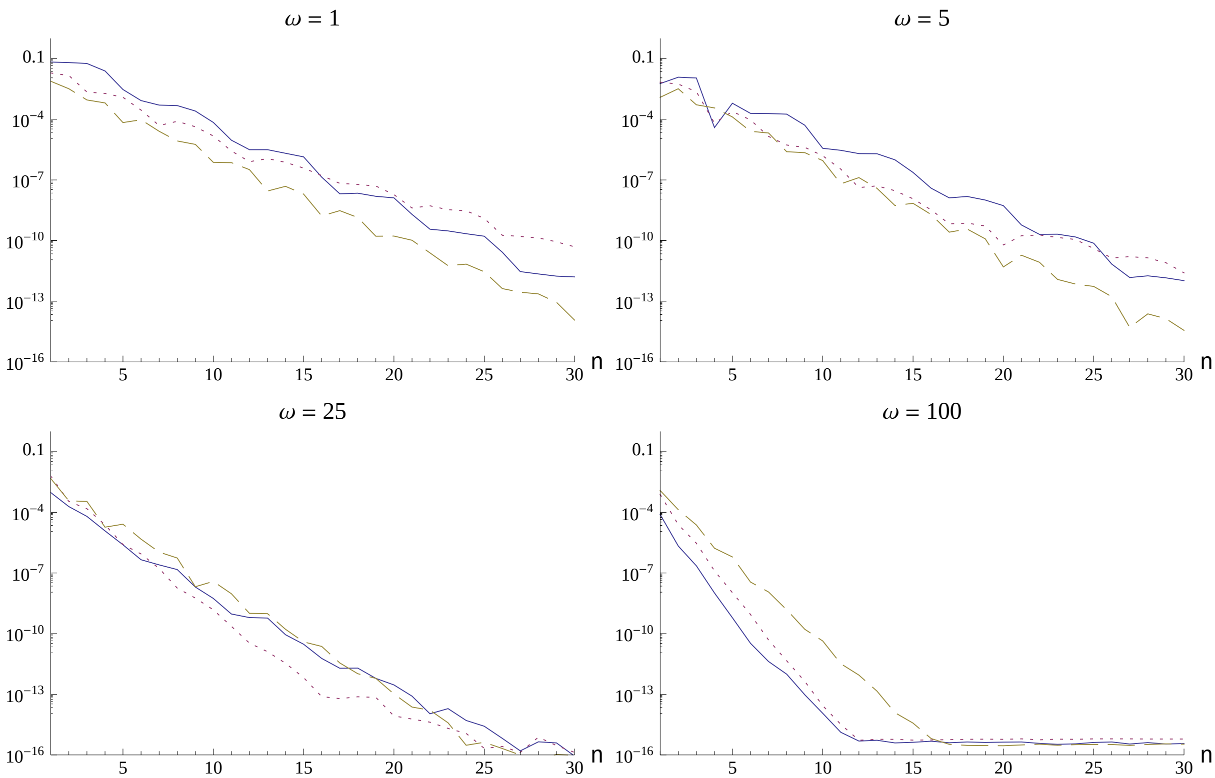

Figure 5: The error in approximating $\int_0^1 \mathrm{e}^{\mathrm{i}kx+\mathrm{i}\omega(x^3+x)}\,\mathrm{d}x$ by $Q_n^{\mathcal{M}}\left[\mathrm{e}^{\mathrm{i}kx}\right]$ for $k = 1$ (plain), 25 (dotted) and 100 (dashed) and four choices of ω.

to ω and/or k increasing) function $\tilde{r}$. Let $f_1 = r_1\mathrm{e}^{\mathrm{i}kp}$ and $f_2 = r_2\mathrm{e}^{\mathrm{i}kp}$ be two functions in $\mathcal{K}_n[\mathcal{M}, f]$. Then their L_2 inner product is

$$\langle f_1, f_2\rangle = \int_a^b r_1\bar{r}_2\mathrm{e}^{\mathrm{i}kp}\mathrm{e}^{-\mathrm{i}kp}\,\mathrm{d}x = \langle r_1, r_2\rangle\,,$$

which is nonoscillatory. In Figure 5 we compute

$$I\left[\mathrm{e}^{\mathrm{i}kx}\right] = \int_0^1 \mathrm{e}^{\mathrm{i}kx+\mathrm{i}\omega(x^3+x)}\,\mathrm{d}x$$

using $Q_n^{\mathcal{M}}\left[\mathrm{e}^{\mathrm{i}kx}\right]$ for twelve choices of ω and k. This demonstrates that the method does not degenerate as k increases, and the rate of convergence still increases with ω.

Unless we are given f and g symbolically, it is not possible to find $\mathcal{M}f$ in closed form. There are several situations where the integrand is indeed given symbolically, for example when applying a spectral method to a specific differential equation, or when computing a special function from its integral representation. As an example of the latter kind, consider the computation of the Airy function, in particular when x is negative and the Airy function is oscillatory. We utilize the integral representation

$$\mathrm{Ai}(x) = \frac{1}{\pi} \int_0^\infty \cos\left(\frac{t^3}{3} + xt\right) \mathrm{d}t. \qquad [\mathbf{1}]$$

We can transform this expression into a form more conducive to differential GMRES, giving us

$$\mathrm{Ai}(x) = \mathrm{Re}\left\{\frac{\sqrt{-x}}{\pi} \int_0^\infty \mathrm{e}^{\mathrm{i}(-x)^{3/2}\left(\frac{t^3}{3}-t\right)} \mathrm{d}t\right\}.$$

We thus define $f(t) = 1$, $g(t) = \frac{t^3}{3} - t$ and $\omega = (-x)^{3/2}$. This integral contains a stationary point at $t = 1$—i.e., $g'(1) = 0$—which is incompatible with the method we have developed. Thus we split the interval into $(0, 2)$ and $(2, \infty)$. On the first interval we could use a Moment-free Filon-type method. As it is outside the scope of this paper, we simply compute the integral over $(0, 2)$ to machine precision, and focus on the latter interval. The integral is free of stationary points in $(2, \infty)$, and hence we employ differential GMRES with the Laguerre inner product

$$\langle p, r\rangle_L = \int_2^\infty p(t)\bar{r}(t)\mathrm{e}^{-t}\,\mathrm{d}t.$$

We now show that the conditions of Theorem 4.5 are satisfied which reveal the asymptotic order of the approximation method. Note that

$$\mathcal{D}\frac{v}{g'} = \mathcal{D}\frac{v}{t^2-1} = \frac{1}{t^2-1}v' - \frac{2t}{(t^2-1)^2}v,$$

hence

$$\mathcal{D}\frac{1}{g'} = -\frac{2t}{(t^2-1)^2}, \quad \left(\mathcal{D}\frac{1}{g'}\right)^2 = 2\frac{1+5t^2}{(t^2-1)^4} \quad \text{and} \quad \left(\mathcal{D}\frac{1}{g'}\right)^3 = -40\frac{t+2t^3}{(t^2-1)^6}.$$

(Here, $\mathcal{D}\frac{1}{g'}$ does not denote an operator, but rather the operator $\mathcal{D}\frac{1}{g'}$ applied to the function 1.) A straightforward inductive argument says that $\left(\mathcal{D}\frac{1}{g'}\right)^k = \mathcal{O}\left(t^{-3k}\right)$. It follows that

$$1 \in \mathcal{B}_{n+1}\left[\mathcal{D}\frac{1}{g'}, \|\cdot\|_L + \left\|\frac{\cdot}{g'}\right\|_\infty + \left\|\mathcal{D}\frac{1}{g'}\cdot\right\|_1\right]$$

for all n. We thus approximate $\mathrm{Ai}(x)$ by

$$\tilde{\mathrm{Ai}}_n(x) = \frac{\sqrt{-x}}{\pi}\mathrm{Re}\left\{\int_0^2 \mathrm{e}^{\mathrm{i}(-x)^{3/2}\left(\frac{t^3}{3}-t\right)} \mathrm{d}t + Q_n^{\mathcal{M}}[1]\right\},$$

which Theorem 4.5 states has an asymptotic order of

$$\mathrm{Ai}(x) - \tilde{\mathrm{Ai}}_n(x) = \mathcal{O}\left(x^{-\frac{3}{2}n-1}\right), \qquad x \to \infty.$$

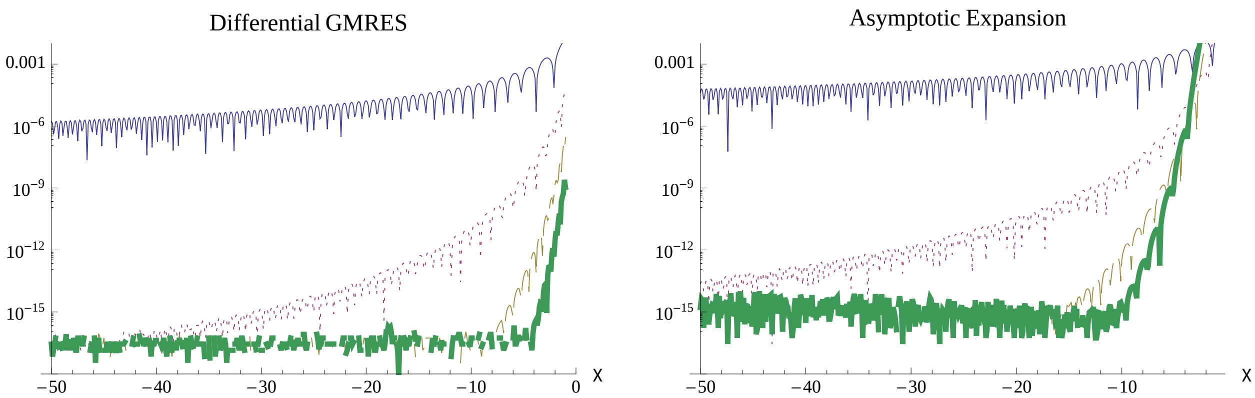

Figure 6: The error in approximating $\mathrm{Ai}(x)$ by $\tilde{\mathrm{Ai}}_n(x)$ (left) and the n-term asymptotic expansion (right) for $n = 1$ (plain), 5 (dotted), 10 (dashed) and 15 (thick).

For any choice of g^{-1}, the analytic continuation of $\frac{1}{g'(g^{-1}(t))}$ has only algebraic growth in the complex plane. Thus $\frac{1}{g'(g^{-1}(t))}\mathrm{e}^{(-x)^{3/2}t}$ decays in the upper half plane for all negative x, and Theorem 3.4 implies that $1 \in \mathcal{G}[\mathcal{M}, \Omega]$. Now convergence in the Laguerre norm follows:

$$\left\|1 - \mathcal{M}v_n^{\mathcal{M}}\right\|_L^2 = \left\|\left|1 - \mathcal{M}v_n^{\mathcal{M}}\right|^2 \mathrm{e}^{-t}\right\|_1 \leq \left\|1 - \mathcal{M}v_n^{\mathcal{M}}\right\|_\infty^2 \left\|\mathrm{e}^{-t}\right\|_1.$$

Perturbing the integration path of $I[1]$ so that it has positive real part suggests that the contribution of the integral over (T, ∞) is super-geometrically small as $T \to \infty$. It should then follow that convergence in the Laguerre norm implies convergence of $\tilde{\mathrm{Ai}}_n(x)$ to $\mathrm{Ai}(x)$, as long as $v_n^{\mathcal{M}}$ does not blow up considerably in a complex neighbourhood of $(2, \infty)$ as $n \to \infty$—a condition which we do not prove. Figure 6 shows the error in the approximation method for four choices of n.

Remark: We needed to increase the precision to 20 digits in Mathematica in order to compute $\mathrm{Ai}(x)$ accurately enough to compare to $\tilde{\mathrm{Ai}}_n(x)$. On the other hand, we only used machine precision arithmetic to compute $Q_n^{\mathcal{M}}[1]$, though we did use 20 digit arithmetic to compute the integral over $(0, 2)$ to machine precision.

There exist many alternative methods for approximating Airy functions for large $|x|$, many based on deformation of the integration contour into the complex plane and integrating along the path of steepest descent. A comprehensive list of algorithms was compiled in [**8**]. In [**3**], Gauss–Laguerre quadrature is utilized along the path of steepest descent, though the error is never compared to the asymptotic expansion, and it is unclear whether high asymptotic orders are achieved. It is instead suggested to switch to the asymptotic expansion whenever $|x|$ is large, for example $|x| \geq 15$. The benefit of our approach is we can use the same method for large and small x, as long as x is bounded away from zero. Furthermore, if

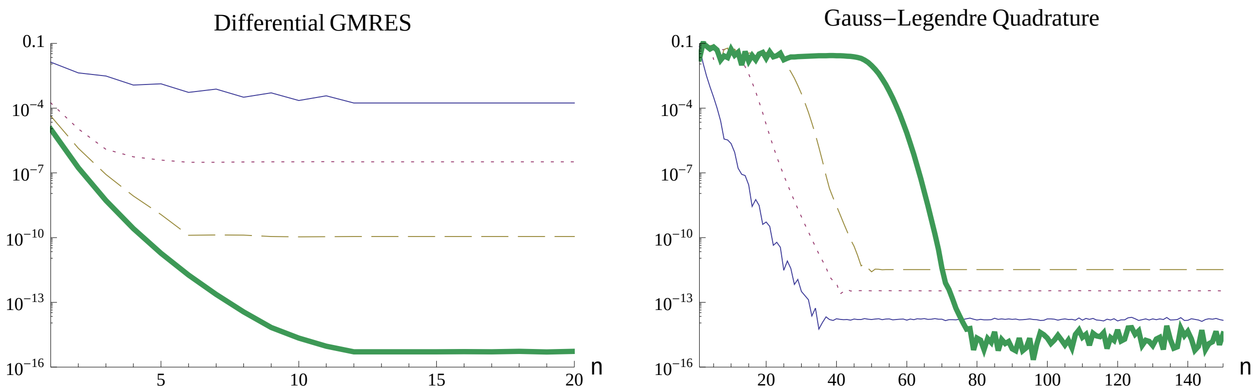

Figure 7: The error in approximating $\int_0^1 \mathrm{e}^{-\frac{1}{x^2}+\mathrm{i}\omega x}\,\mathrm{d}x$ by $Q_n^{\mathcal{M}}[f]$ (left) and an n-point Gauss–Legendre rule (right), for $\omega = 1$ (plain), 50 (dotted), 100 (dashed) and 200 (thick).

more than machine precision is required, the accuracy of asymptotic expansions is limited, whereas $\tilde{\mathrm{A}}\mathrm{i}_n$ is arbitrarily accurate.

Using the property that $Q_n^{\mathcal{M}}[f]$ remains accurate in the complex plane—demonstrated in Figure 4—presents the intriguing possibility that a uniform approximation to the Airy function throughout the complex plane can be found. Whether complications arising from the change of variables and choice of integration path can be overcome has yet to be investigated.

All examples so far have utilized analytic functions, and seem to roughly achieve super-algebraic convergence. On the other hand, if f is only $\mathbb{C}^r$, convergence is impossible: the Krylov subspace depends on derivatives and is no longer well-defined. This leaves one other possible set of functions f for which we can use this approximation method: functions which are $\mathbb{C}^\infty$ but not analytic. Thus consider the integral

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

This has a single point where analyticity is lost: at $x = 0$. Unfortunately, it seems in Figure 7 that convergence to the exact solution is no longer achieved, though the asymptotic decay rate is still maintained due to Theorem 4.5, which never utilized analyticity. If we choose an integration range that does not contain zero, then convergence is again guaranteed.

6. Closing remarks

We have presented a new method for computing oscillatory integrals that captures the asymptotic decay of the asymptotic expansion, and in some sense converges uniformly throughout the complex plane. Furthermore, it remains accurate when the integrand has oscillations at multiple scales. The method shows potential for computing uniform approximations to special functions with integral representations.

Since the method is based on finding a particular solution to a first order differential equation, it raises the possibility of generalizing differential GMRES to compute higher order ordinary, or even partial, differential equations. There are several additional complications in these situations which must be overcome, for example imposing initial or boundary conditions and proving convergence.

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