THE INFINITE ARNOLDI EXPONENTIAL INTEGRATOR FOR LINEAR INHOMOGENEOUS ODES

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Abstract. Exponential integrators that use Krylov approximations of matrix functions have turned out to be efficient for the time-integration of certain ordinary differential equations (ODEs). This holds in particular for linear homogeneous ODEs, where the exponential integrator is equivalent to approximating the product of the matrix exponential and a vector. In this paper, we consider linear inhomogeneous ODEs, \( y'(t) = Ay(t) + g(t) \), where the function \( g(t) \) is assumed to satisfy certain regularity conditions. We derive an algorithm for this problem which is equivalent to approximating the product of the matrix exponential and a vector using Arnoldi’s method. The construction is based on expressing the function \( g(t) \) as a linear combination of given basis functions \( \phi_i \) with particular properties. The properties are such that the inhomogeneous ODE can be restated as an infinite-dimensional linear homogeneous ODE. Moreover, the linear homogeneous infinite-dimensional ODE has properties that directly allow us to extend a Krylov method for finite-dimensional linear ODEs. Although the construction is based on an infinite-dimensional operator, the algorithm can be carried out with operations involving matrices and vectors of finite size. This type of construction resembles in many ways the infinite Arnoldi method for nonlinear eigenvalue problems \[15\]. We prove convergence of the algorithm under certain natural conditions, and illustrate properties of the algorithm with examples stemming from the discretization of partial differential equations.

Key words. Arnoldi’s method, exponential integrators, matrix functions, ordinary differential equations, Bessel functions

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1. Introduction. Consider a matrix \( A \in \mathbb{C}^{n \times n} \) and a function \( g: \mathbb{C} \rightarrow \mathbb{C}^n \) with elements which are entire functions. We consider the problem of numerically computing the time-evolution of the linear ordinary differential equation with an inhomogeneous term

\[
u'(t) = Au(t) + g(t), \quad u(0) = u_0. \tag{1.1}\]

Our focus will be on equations that arise from spatial semidiscretization of partial differential equations of evolutionary type, and \( A \) will typically be a large sparse matrix, and \( g \) will neither be close to linear nor correspond to an extremely stiff nonlinearity, in a sense which is further explained in the examples in Section \[5\].

The general problem of computing the time-evolution of ODEs can be approached with various numerical methods. The method we will present in this paper belongs to the class of methods called exponential integrators. Exponential integrators have recently received considerable interest; see the review paper \[14\]. An attractive feature of these methods stems from the combination of approximation of matrix functions and the use of Krylov methods \[13\]. This is mostly due to the superlinear convergence of the Krylov approximation of entire matrix functions \[12\].

In this paper we will present a new exponential integrator for \([14]\). The integrator is constructed using a particular type of expansion of the function \( g \) in \([14]\). We will

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consider expansions of the type

$$g(s) = \sum_{\ell=0}^{\infty} w_{\ell} \phi_{\ell}(s),$$  \hspace{1cm} (1.2)

where $w_{\ell} \in \mathbb{C}^n$, $\ell \in \mathbb{N}$, and the basis functions $\phi_0, \phi_1, \ldots$ are assumed to satisfy

$$\frac{d}{dt} \begin{bmatrix} \phi_0(t) \\ \phi_1(t) \\ \vdots \end{bmatrix} = H_{\infty} \begin{bmatrix} \phi_0(t) \\ \phi_1(t) \\ \vdots \end{bmatrix}, \quad \begin{bmatrix} \phi_0(0) \\ \phi_1(0) \\ \vdots \end{bmatrix} = e_1$$  \hspace{1cm} (1.3a)

where $H_{\infty} \in \mathbb{R}^{\infty \times \infty}$ is an infinite-dimensional Hessenberg matrix, satisfying for a fixed constant $C \geq 0$,

$$\|H_N\| < C \text{ for all } N = 0, \ldots, \infty. \hspace{1cm} (1.3b)$$

The matrix $H_N \in \mathbb{R}^{N \times N}$ is the leading submatrix of $H_{\infty}$.

The scaled monomials is the easiest example of such a sequence of functions. If we define $\phi_{i}(t) := t^i / i!$, $i = 0, \ldots$, then (1.3) is satisfied with $H_{\infty}$ given by a transposed Jordan matrix

$$H_{\infty} = \begin{bmatrix} 0 & 1 & 0 & \cdots \\ 1 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \\ \end{bmatrix}. \hspace{1cm} (1.4)$$

In this case, the expansion (1.2) corresponds to a Taylor expansion and the coefficients are given by $w_{\ell} = g^{(\ell)}(0)$, $\ell = 0, \ldots$. We will also see that these properties are satisfied for other functions, e.g., the Bessel function and the modified Bessel function of the first kind (as we will further explain in Section 2.2). The algorithm will be derived and analyzed for these choices of $[\phi_i]_{i=0}^{\infty}$. The choice of basis functions can be tailored for the problem, and the best choice is problem dependent. This will be illustrated in the numerical examples in Section 5.

The general idea of our approach can be seen as follows. If $\phi_0, \phi_1, \ldots$ are the scaled monomials, then we can truncate (1.2) at $\ell = N$, yielding $\tilde{y}(t) = A\tilde{y}(t) + \sum_{\ell=0}^{N-1} w_{\ell} \phi_{\ell}(t)$ and it straightforward to verify that the inhomogeneous ODE (1.1) can be expressed as a larger linear homogeneous ODE,

$$\frac{d}{dt} \begin{bmatrix} \tilde{y}(t) \\ \phi_0(t) \\ \vdots \\ \phi_{N-1}(t) \end{bmatrix} = A_N \begin{bmatrix} \tilde{y}(t) \\ \phi_0(t) \\ \vdots \\ \phi_{N-1}(t) \end{bmatrix}, \quad \begin{bmatrix} y(0) \\ \phi_0(0) \\ \vdots \\ \phi_{N-1}(0) \end{bmatrix} = \begin{bmatrix} y_0 \\ e_1 \end{bmatrix}$$  \hspace{1cm} (1.5)

where we have defined

$$A_N := \begin{bmatrix} A & W_N \\ 0 & H_N \end{bmatrix} \hspace{1cm} (1.6)$$

and $H_N \in \mathbb{R}^{N \times N}$ is the leading $N \times N$ block of $H_{\infty}$ and $W_N := [w_0 \cdots w_{N-1}] \in \mathbb{C}^{n \times N}$. This relation has been used in [2, Theorem 2.1] and also in [16]. If we combine this type of construction with an iterative method (in a particular way), we will here...
be able to construct an algorithm for (1.1) for any sequence of functions \( \phi_0, \phi_1, \ldots \) satisfying (1.3).

The construction (1.3) and the matrix (1.0) resemble in some ways the technique called companion linearization used for polynomial eigenvalue problems; see e.g. [17, 21]. The algorithm known as the infinite Arnoldi method [15] is an algorithm for nonlinear eigenvalue problems (not necessarily polynomial). One variant of the infinite Arnoldi method can be interpreted as the Arnoldi method [20] applied to the companion linearization of a truncated Taylor expansion. Due to a particular structure of the companion matrix, the infinite Arnoldi method is also equivalent to the application of the Arnoldi method on an infinite-dimensional companion matrix. This equivalence is consistent with the observation that many attractive features of the Arnoldi method appear to be present also in the infinite Arnoldi method.

We will in this paper illustrate that the underlying techniques used to derive the infinite Arnoldi method can also be applied to (1.1). Similar to the infinite Arnoldi method, the presented algorithm can be interpreted as an exponential integrator applied to a truncated problem, as well as the integrator applied to an infinite-dimensional problem. An important feature of this construction is that the algorithm does not require a choice of a truncation parameter in the expansion (1.2), making it in a sense applicable to arbitrary nonlinearities.

The paper is structured as follows. The infinite-dimensional properties of the algorithm are derived in Section 2.1. Although the construction in Section 2.1 is general for essentially arbitrary basis, the convergence proofs are basis dependent. We show that the algorithm converges for several bases (scaled monomials, Bessel functions and modified Bessel functions) under certain conditions, i.e., the truncation of (1.2) converges and the derivatives \( g^{(i)}(0) \) of the nonlinearity are bounded with respect to the linear operator \( A \) in a certain way. This convergence theory is presented in Section 4. We illustrate the properties of the algorithm and its variants in Section 5 including comparisons with other algorithms.

We will mostly use standard notation. \((H_N)_{i,j}\) denotes the element at the \( i \)th row and \( j \)th column of \( H_N \). Analogously, the colon notation will be used to denote entire rows and columns, e.g., \( V_k : \) corresponds to the vector in the \( k \)th row of the matrix \( V \). We will also extensively use infinite-dimensional matrices. More precisely, we will work with sequences of matrices \( W_N \in \mathbb{R}^{n \times N} \), \( N = 0, \ldots \), which are nested, i.e., \( W_{N-1} \in \mathbb{R}^{n \times (N-1)} \) are the first \( N - 1 \) columns of \( W_N \), and \( W_\infty \) will be the corresponding infinite-dimensional matrix. We will also consider sequences of square matrices \( H_N \in \mathbb{R}^{N \times N} \), where \( H_{N-1} \) is the leading submatrix of \( H_N \). The infinite-dimensional operator associated with the limit will be denoted \( H_\infty \in \mathbb{R}^{\infty \times \infty} \). We will use \( e_i \) to denote the \( i \)th unit vector of consistent size. Throughout the paper, \( \| \cdot \| \) denotes the Euclidean vector norm or the spectral matrix norm, unless otherwise stated.

2. Preliminaries.

2.1. Infinite-dimensional reformulation. At first we will show that the inhomogeneous ODE (1.1) is equivalent to an infinite-dimensional homogeneous ODE. The reformulation is illustrated in the following lemma and can be interpreted as an analogous transformation illustrated for monomials and truncated Taylor expansion in (1.3) and (1.0), but without truncation and for arbitrary basis functions satisfying (1.3).
Lemma 1 (Infinite-dimensional reformulation) Consider the initial value problem \((1.1)\), and a sequence of basis functions \([\phi_i]_{i=0}^{\infty}\) which satisfy \((1.3)\). Moreover, suppose that the function \(g\) in \((1.1)\) can be expanded as \((1.2)\), and let \(W_\infty = [w_0, w_1, w_2, \ldots] \in \mathbb{C}^{n \times \infty}\) denote the expansion coefficients.

(a) Suppose \(u(t)\) is a solution to \((1.1)\). Then
\[
\frac{d}{dt} \begin{bmatrix} u \\ \phi_0 \\ \vdots \end{bmatrix} = \begin{bmatrix} A & W_\infty \\ 0 & H_\infty \end{bmatrix} \begin{bmatrix} u \\ \phi_0 \\ \vdots \end{bmatrix}, \quad \begin{bmatrix} u(0) \\ \phi_0(0) \\ \vdots \end{bmatrix} = \begin{bmatrix} u_0 \\ e_1 \end{bmatrix}. \tag{2.1}
\]

(b) Suppose \(v(t)\) satisfies
\[
v'(t) = \begin{bmatrix} A & W_\infty \\ 0 & H_\infty \end{bmatrix} v(t), \quad v(0) = \begin{bmatrix} u_0 \\ e_1 \end{bmatrix}. \tag{2.2}
\]

Then the function \(u(t) := \begin{bmatrix} I_n & 0 \end{bmatrix} v(t)\) is the unique solution to \((1.1)\).

Proof. The equation \((2.1)\) is easily verified by considering the individual blocks. The first \(n\) rows of \((2.1)\) satisfy \(u'(t) = Au(t) + \sum_{i=0}^{\infty} W_i \phi_i(t) = Au(t) + g(t)\). Rows \(n+1, n+2, \ldots\) are precisely the conditions in \((1.3)\). In order to show \((2.2)\), first note that the rows \(n+1, n+2, \ldots\) in \((2.2)\) reduce to the equation
\[
\frac{d}{dt} \begin{bmatrix} v_{n+1}(t) \\ \vdots \\ v_n(0) \end{bmatrix} = H_\infty \begin{bmatrix} v_{n+1}(t) \\ \vdots \\ v_n(0) \end{bmatrix} = e_1.
\]

Since the operator \(H_\infty\) has a finite norm by assumption \((1.3)\), it follows from the Picard-Lindelöf theorem that there exists a unique solution. This solution is the sequence of basis functions \(\phi_0, \phi_1, \ldots\), since they satisfy this ODE by assumption, i.e., \(v_{n+1+i} = \phi_i\) for all \(i \in \mathbb{N}\). The conclusion follows by substituting \(v(t)\) into the first \(n\) rows in \((2.2)\). 

2.2. Characterization of basis functions \(\phi_i\). As mentioned in the introduction (in particular in formula \((1.4)\)), it is straightforward to verify that the scaled monomials satisfy the condition \((1.3)\) required for the basis functions. Although the algorithm described in the following section applies for any basis functions satisfying \((1.3)\), we will concentrate the discussion on specialized results for two additional types of functions. We will now show that the Bessel functions and the modified Bessel functions of the first kind satisfy \((1.3)\).

The Bessel functions of the first kind are defined by (see e.g. \([1]\)),
\[
J_\ell(t) := \frac{1}{\pi} \int_0^\pi \cos(\ell \tau - t \sin(\tau)) \, d\tau, \quad \ell \in \mathbb{N},
\]
and they satisfy
\[
J_\ell(0) = \begin{cases} 
1 & \text{if } \ell = 0 \\
0 & \text{otherwise} 
\end{cases}. \tag{2.3c}
\]

Let \(J_N(t) = [J_0(t) \quad J_1(t) \quad \ldots \quad J_{N-1}(t)]^T \in \mathbb{R}^N\), i.e., a vector of Bessel functions.
with non-negative index. Moreover, let

\[
H_N = \begin{bmatrix}
0 & -1 & & & \\
\frac{1}{2} & 0 & -\frac{1}{2} & & \\
& \ddots & \ddots & \ddots & \\
\vdots & & \ddots & \ddots & \\
& & & 0 & -\frac{1}{2} \\
& & & \frac{1}{2} & 0
\end{bmatrix} \in \mathbb{C}^{N \times N}.
\] (2.4)

From the relations (2.3), we easily verify that the Bessel functions of the first kind are solutions to the infinite-dimensional ODE of the form (1.3), with \(H_N\) given by (2.4). More precisely,

\[
\bar{J}_\infty'(t) = H_\infty \bar{J}_\infty(t), \quad \bar{J}_\infty(0) = e_1.
\]

With similar reasoning we can establish an ODE (1.3) also for the modified Bessel functions of the first kind, which are defined by

\[
I_\ell(t) := (-i)^n J_n(it).
\] (2.5)

and satisfy \(I'_\ell(t) = \frac{1}{2}(I_{\ell-1}(t) + I_{\ell+1}(t)), \ell \in \mathbb{N}\). These properties lead to the infinite-dimensional ODE

\[
\bar{I}_\infty'(t) = H_\infty \bar{I}_\infty(t), \quad I(0) = e_1,
\]

where \(\bar{I}_N(t) = [I_0(t) \quad I_1(t) \quad \ldots \quad I_{N-1}(t)]^T\) and

\[
H_N = \begin{bmatrix}
0 & 1 & & & \\
\frac{1}{2} & 0 & \frac{1}{2} & & \\
& \ddots & \ddots & \ddots & \\
\vdots & & \ddots & \ddots & \\
& & & 0 & \frac{1}{2} \\
& & & \frac{1}{2} & 0
\end{bmatrix} \in \mathbb{C}^{N \times N}.
\] (2.6)

Therefore, we can show that the Bessel functions and the modified Bessel functions of the first kind satisfy (1.3), with an explicitly given constant \(C\).

**Lemma 2 (Basis functions)** The conditions for the basis functions in (1.3) are satisfied with \(C = 2\) for,

(a) scaled monomials, i.e., \(\phi_i(t) = t^i/i!\), with \(H_\infty\) defined by (1.4);

(b) Bessel functions, i.e., \(\phi_i(t) = J_i(t)\), with \(H_\infty\) defined by (2.4); and

(c) modified Bessel functions, i.e., \(\phi_i(t) = I_i(t)\), with \(H_\infty\) defined by (2.6).

**Proof.** Statement (a) follows from the definition. The conditions (1.3a) have been shown already for (b) and (c), since they follow directly from (2.3) and (2.5). It remains to show that the uniform bound (1.3b) is satisfied for (b) and (c). Note that in both cases (b) and (c) we can express \(H_N\) as \(H_N = T_N + E_N\), where \(E_N = \pm \frac{1}{2} e_1 e_2^T\) and \(T_N\) is a (finite) band Toeplitz matrix, for any \(N = 2, \ldots, \infty\). We now invoke a general result for (finite) band Toeplitz matrices [5, Theorem 1.1] which implies that

\[
\|T_N\| \leq \|T_\infty\| = 1.
\]

Hence, \(\|H_N\| \leq \|T_N\| + \|E_N\| = 3/2\), and (1.3a) holds with \(C = 2\). \(\square\)
2.3. Characterization of expansion coefficients $w_\ell$. In principle, the algorithm will be applicable to any problem for which there is a convergent expansion of the form (1.2) with some coefficients $w_\ell \in \mathbb{C}$, $\ell \in \mathbb{N}$. In practice these coefficients may not be explicitly available. We will now characterize a relationship between the coefficients and the derivatives of $g$. This will be necessary in the theoretical convergence analysis in Section 4 and also useful in numerical evaluation of the coefficients (Section 5).

Assume that an expansion of the form (1.2) exists and let

$$W_N = [w_0 \ w_1 \ldots \ w_{N-1}] .$$

By considering the $l$th derivative of $g(t)$ and using the properties of basis functions (1.3) we have that

$$g^{(l)}(0) = W_\infty H_\infty^l e_1 = W_N H_N^l e_1 \quad \text{for all} \quad l < N .$$

In the last equality we used the fact that $H_\infty$ is a Hessenberg matrix, and that all elements of $H_\infty^l e_1$ except the first $l + 1$ elements will be zero. The non-zero elements will also be equal to $H_N^l e_1$. We now define the upper-triangular matrix

$$K_N(H_N, e_1) = [e_1 \ H_N e_1 \ldots \ H_N^{N-1} e_1] , \quad (2.7)$$

and the matrix $G_N$ as

$$G_N = [g(0) \ g'(0) \ldots \ g^{(N-1)}(0)] . \quad (2.8)$$

From the definition it follows that

$$W_N = G_N K_N(H_N, e_1)^{-1} \quad \text{for all} \quad N \geq 1 , \quad (2.9)$$

under the condition that $K_N(H_N, e_1)$ is invertible. In a generic situation, the relation (2.9) can be directly used to compute the coefficients $w_\ell$, $\ell \in \mathbb{N}$, given the derivatives of $g(t)$. For the Bessel functions and the modified Bessel functions of the first kind, we can characterize the coefficients with a more explicit (and more numerically robust) formula involving the monomial coefficients of the Chebyshev polynomials of the first kind.

**Lemma 3** Let $T_{k,\ell}$ be the monomial coefficients of the $k$th Chebyshev polynomial, i.e., $T_k(x) = \sum_{\ell=0}^{k} T_{k,\ell} x^\ell$.

(a) For scaled monomials, i.e., $\phi_k(t) = t! / k!$, the expansion coefficients are given by $w_k = g^{(k)}(0)$, for $k \in \mathbb{N}$.

(b) For the Bessel functions of the first kind, i.e., $\phi_\ell(t) = J_\ell(t)$, the expansion coefficients $w_\ell$ are given by,

$$w_0 = g(0) , \quad w_k = 2^k \sum_{\ell=0}^{k} (-1)^\ell T_{k,\ell} g^{(\ell)}(0) , \quad k = 1 , \ldots .$$

(c) For the modified Bessel functions of the first kind, i.e., $\phi_\ell(t) = I_\ell(t)$, the expansion coefficients $w_\ell$ are given by,

$$w_0 = g(0) , \quad w_k = 2^k \sum_{\ell=0}^{k} T_{k,\ell} g^{(\ell)}(0) , \quad k = 1 , \ldots .$$
Proof. Case (a) follows from the definition. Consider case (c) with the modified Bessel functions, i.e., let \( H_N \) be given by (2.6). The proof is based on showing that

\[
K_N(H_N, e_1)^{-1} = \begin{bmatrix}
\frac{1}{2}T_{0,0} & T_{1,0} & \cdots & T_{N-1,0} \\
0 & T_{1,1} & & T_{N-1,1} \\
\vdots & \ddots & \ddots & \vdots \\
0 & & \cdots & T_{N-1,N-1}
\end{bmatrix},
\]

from which the conclusion follows directly from (2.9) and the fact that \( T_{k,k} = 2^{k-1} \) for any \( k > 0 \).

We will first prove (2.10) for columns \( k = 2, 3, \ldots, N \). From (2.7) and (2.6) we directly identify that

\[
K_{N+1}(H_{N+1}, e_1) = \begin{bmatrix}
K_N(H_N, e_1) & H_N^N e_1 \\
0 & 2^{-N}
\end{bmatrix}.
\]

Moreover, by explicitly formulating the Schur complement [8, Section 3.2.11] we have that

\[
K_{N+1}(H_{N+1}, e_1)^{-1} = \begin{bmatrix}
K_N(H_N, e_1)^{-1} & -2^N K_N(H_N, e_1)^{-1} H_N^N e_1 \\
0 & 2^{-N}
\end{bmatrix}.
\]

Now let \( p_N(\lambda) \) be the characteristic polynomial of \( H_N \), i.e., \( p_N(\lambda) = \det(\lambda I - H_N) \).

By expanding the determinant of \( \lambda I - H_N \) for the last row, we find that

\[
p_N(\lambda) = \lambda p_{N-1}(\lambda) - \frac{1}{4} p_{N-2}(\lambda).
\]

Now let \( \tilde{p}_N(\lambda) := 2^{N-1} p_N(\lambda) \) which satisfies the recursion \( \tilde{p}_N(\lambda) = 2\lambda \tilde{p}_{N-1}(\lambda) - \tilde{p}_{N-2}(\lambda) \). This is exactly the recursion of the Chebyshev polynomials. We have \( \tilde{p}_1(\lambda) = \lambda = T_1(\lambda) \) and \( \tilde{p}_2(\lambda) = (2\lambda^2 - 1) = T_2(\lambda) \). Hence, by induction starting with \( N = 1 \) and \( N = 2 \) it follows that \( \tilde{p}_N(\lambda) = T_N(\lambda) \), for all \( N \geq 1 \). Note that \( \tilde{p}_0 \neq 0 \).

The Cayley-Hamilton theorem implies that \( 0 = p_N(H_N) = \tilde{p}_N(H_N) = T_N(H_N) \) and in particular \( 0 = 2\tilde{p}(H_N)e_1 \), i.e.,

\[
-2^N \tilde{H}_N^N e_1 = \sum_{i=0}^{N-1} 2T_{N,i} H_N^i e_1.
\]

The first \( N \) rows of the last column of (2.11) can now be expressed as

\[
-2^N K_N(H_N, e_1)^{-1} H_N^N e_1 = 2K_N(H_N, e_1)^{-1} \left( \sum_{i=0}^{N-1} T_{N,i} H_N^i e_1 \right) = 2 \begin{bmatrix}
T_{N,0} \\
\vdots \\
T_{N,N-1}
\end{bmatrix}
\]

The structure in (2.10) for columns \( k = 2, \ldots, N \) follows by induction. The first column can be verified directly by noting that \( K_1(H_1, e_1) = 1 = T_{0,0} \).

The proof for the case (b) goes analogously. From (2.6) we see that in this case the characteristic polynomial \( p_N(\lambda) \) of \( H_N \) satisfies the recursion

\[
p_N(\lambda) = \lambda p_{N-1}(\lambda) + \frac{1}{4} p_{N-2}(\lambda).
\]

Defining \( \tilde{p}_N(\lambda) = 2^{N-1} p_N(\lambda) \) and writing out the recursions we find (similarly to the case (c)) that \( \tilde{p}_N(\lambda) = (-1)^N T_N(\lambda) \). Comparing (2.12) and (2.14) we see that \( \tilde{p}_N(\lambda) \) is of the form \( \tilde{p}_N(\lambda) = \sum_{i=0}^N |T_{N,i}| \lambda^i \). The claim follows from this. \( \square \)
Remark 4 (Combining with formulas for the Chebyshev polynomials) The coefficients $T_{k,\ell}$ are given by the explicit expression (see [1, pp. 775])

$$T_k(x) = \left\lfloor \frac{k}{2} \right\rfloor \sum_{\ell=0}^{\left\lfloor k/2 \right\rfloor} (-1)^{\ell} \frac{k!}{\ell!(k-2\ell)!} 2^{k-2\ell-1} x^{k-2\ell}. \quad (2.15)$$

Thus, when the basis functions $\phi_\ell$ are the modified Bessel functions of the first kind, the coefficients of the expansion (1.2) are explicitly given by

$$w_k = \left\lfloor \frac{k}{2} \right\rfloor \sum_{\ell=0}^{\left\lfloor k/2 \right\rfloor} (-1)^{\ell} \frac{k!}{\ell!(k-2\ell)!} 2^{k-2\ell-1} g^{(k-2\ell)}$$

$$= \sum_{\ell=0}^{\left\lfloor k/2 \right\rfloor} (-1)^{\ell} \frac{k!}{\ell!(k-2\ell)!} 2^{k-2\ell-1} \left( \frac{1}{2\pi i} \int_{\Gamma} g(\lambda) \lambda^{k-2\ell} d\lambda \right), \quad (2.16)$$

where in the last step we have used the Cauchy integral formula. For the expansions with the Bessel functions of the first kind we get exactly the same formula, with $(-1)^{\ell}$ replaced by 1 in the summand, which is also given in [24, Sec. 9.1].

3. Infinite Arnoldi exponential integrator for (1.1). Consider for the moment a linear (finite-dimensional) homogeneous ODE

$$y'(t) = By(t), \quad y(0) = b \quad (3.1)$$

where $y(t) \in \mathbb{C}^n$, with the solution given by the matrix exponential $y(t) = \exp(tB)b$. Algorithms for (3.1) based on Krylov methods are typically constructed as follows, see [11] and references therein for further details. By carrying out $N$ steps of the Arnoldi process for $B$ and $b$ we obtain the Hessenberg matrix $F_N$ and the orthonormal matrix $Q_N \in \mathbb{C}^{n \times (N+1)}$ that satisfy the so called Arnoldi relation

$$BQ_N = Q_N F_N + f_{N+1} q_{N+1} e_N^T, \quad (3.2)$$

where $q_i$ denotes the $i$th column of $Q_{N+1} = [q_1, \ldots, q_{N+1}] = [Q_N, q_{N+1}]$ and $f_{i,j}$ the $i,j$ element of $F_N$, and $q_1 = b/\beta$ with $\beta := \|b\|$. The columns of $Q_N$ form an orthogonal basis of the Krylov subspace

$$K_N(B, b) = \text{span}(b, Bb, \ldots, B^{N-1}b).$$

As a consequence of (3.2), the Hessenberg matrix $F_N$ is the projection of $B$ onto the Krylov subspace $K_N(B, b)$, i.e., $F_N = Q_N^T B Q_N$.

The Krylov approximation of (3.1) is subsequently given by

$$y(t) = \exp(tB)b \approx Q_N \exp(tF_N) e_1 \beta. \quad (3.3)$$

Krylov approximations of the matrix exponential has for instance been used in [6, 18, 23].

The first justification of the proposed algorithm is based on applying a Krylov approximation analogous to (3.3) for the infinite-dimensional homogeneous ODE given in Lemma 1. Although this construction is infinite-dimensional, it turns out that due to the structure of $A_\infty$ and the starting vector $b = [u_0^T, e_1^T]^T \in \mathbb{C}^\infty$, the basis matrix $Q_N$ has a particular structure which can be exploited.
Lemma 5 (Basis matrix structure) Let \( Q_N \in \mathbb{C}^{\infty \times N} \) be the matrix generated by the Arnoldi method applied to the infinite matrix \( A_\infty \) given by (1.6) and the starting vector \( b = [u_0^T, e_1^T]^T \in \mathbb{C}^\infty \). Let \( q_{1,j} \in \mathbb{C}^{n+1} \), for \( j = 1 \ldots N \), be the first \( n+1 \) rows of \( Q_N \) and let \( q_{i,j} \in \mathbb{C}^n \), for \( i = 2, \ldots, j = 2, \ldots, N \), correspond to the rows \( n+2, n+3, \ldots \).

Then, the basis matrix \( Q_N \) has the block-triangular structure

\[
Q_N = \begin{bmatrix}
q_{1,1} & q_{1,2} & \cdots & q_{1,N} \\
0 & q_{2,2} & \cdots & q_{2,N} \\
\vdots & 0 & \ddots & \vdots \\
\vdots & 0 & q_{N,N} \\
\vdots & 0 & \cdots & 0 \\
\end{bmatrix} \in \mathbb{C}^{\infty \times N} \tag{3.4}
\]

Proof. The proof can be done by induction. For \( N = 1 \) the statement is trivial. If we assume \( Q_N \) has the structure (3.4), at step \( N \) the Arnoldi method will generate a new vector \( q_{N+1} \in \mathbb{C}^\infty \) which is a linear combination of \( A_\infty q_{N} \) and the columns of \( Q_N \). Due to the fact that \( H_\infty \) is a Hessenberg matrix, and \( A_\infty \) has the structure (1.6), \( A_\infty q_{N} \) will have one more non-zero element than \( q_{N} \). This completes the proof.

The zero-structure in the basis matrix \( Q_N \) revealed in Lemma 5 suggests that we can implement the Arnoldi method for (2.2) by only storing the non-zero part of \( Q_N \). By noting that the orthogonalization also preserves the basis matrix structure, we can derive an algorithm where in every step the basis matrix is expanded by a column and a row. We note that the infinite Arnoldi method for nonlinear eigenvalue problems has a similar property [15, Section 5.1]. The proposed algorithm is specified in Algorithm 1. As is common for the Arnoldi method, in Step \( 7 \) we used reorthogonalization if necessary.

Another natural procedure to compute a solution to (1.1) would be to truncate the matrix \( H_\infty \) and thereby \( A_\infty \) such that we obtain a linear finite-dimensional ODE

\[
\tilde{v}'(t) = A_m \tilde{v}(t), \quad \tilde{v}(0) = \begin{bmatrix} u_0 \\ e_1 \end{bmatrix}
\]

using (1.5) and subsequently applying the standard Krylov approximation (3.3) on this finite-dimensional ODE. It turns out that this approach will provide an algorithm equivalent to Algorithm 1 if the truncation parameter is chosen larger or equal to the number of Arnoldi steps. Hence, in addition to the fact that Algorithm 1 can be interpreted as an infinite-dimensional Krylov approximation of (2.2), the algorithm is also equivalent to the finite-dimensional Krylov approximation corresponding to the truncated matrix, if the truncation parameter is chosen larger than the number of steps.

Lemma 6 Consider \( N \) steps of the Arnoldi method applied to \( A_m \in \mathbb{C}^{(n+m) \times (n+m)} \) with starting vector \( b = [u_0^T, e_1^T]^T \in \mathbb{C}^{n+m} \). Let \( u_{N,m} \) be the corresponding Krylov approximation, i.e., \( u_{N,m} := [I_n \quad 0] Q_N \exp(tF_N) e_1 \beta \). Then, for any \( m \geq N \), we have \( u_{N,m} = u_{N,m} \).

Proof. This follows directly from the zero-structure of the basis matrix in (3.4), which holds also for finite \( m \), when \( m \geq N \).
Algorithm 1: The infinite Arnoldi exponential integrator for (1.1)

Input: \( u_0 \in \mathbb{C}^n, t \in \mathbb{R}, w_0, w_1, \ldots \in \mathbb{C}^n \)

output: The approximation \( u_{IA}^N \approx u(t) \)

1. Let \( \beta = \|u_0\| \), \( Q_1 = u_0/\beta \), \( F_0 = \text{empty matrix} \)

for \( k = 1, 2, \ldots, N \) do

2. Let \( q_k = Q(:, k) \in \mathbb{C}^{n+k-1} \)

3. Compute \( w := A_k q_k \)

4. Let \( \tilde{Q}_k \) be \( Q_k \) with one zero row added

5. Compute \( h = \tilde{Q}_k^* w \)

6. Compute \( w_\perp := w - \tilde{Q}_k h \)

7. Repeat Step 5-6 if necessary

8. Compute \( \alpha = \|w_\perp\| \)

9. Let \( F_k = \begin{bmatrix} F_{k-1} & h \\ 0 & \alpha \end{bmatrix} \)

10. Let \( Q_{k+1} := [Q_k, w_\perp/\alpha] \)

end

11. Let \( F_N \in \mathbb{R}^{N \times N} \) be the leading submatrix of \( F_N \in \mathbb{R}^{(N+1) \times N} \)

12. Compute the approximation \( u_{IA}^N = [I_n \ 0] Q_N \exp(tF_N)e_1 \beta \)

4. Convergence analysis. We saw in Lemma 6 that although the Algorithm 1 is derived from Arnoldi’s method applied to an infinite-dimensional operator \( A_\infty \), the result of \( N \) steps of the algorithm can also be interpreted as Arnoldi’s method applied to the truncated matrix \( A_m \) for any \( m \leq N \). In order to study the convergence we will set \( m = N \) and use the exact solution associated with the truncated matrix \( A_N \), denoted by \( u_N(t) \). More precisely,

\[
   u_N(t) := [I_n \ 0] \exp(tA_N)u_N. \tag{4.1}
\]

By trivial subtraction and triangle inequality we have that the error is bounded by

\[
   \|u^A_{IA} - u(t)\| \leq \|u(t) - u_N(t)\| + \|u_N(t) - u^A_{IA}\|. \tag{4.2}
\]

The first term \( \|u(t) - u_N(t)\| \) can be interpreted as an error associated with \( A_N \) (the truncation of \( A_\infty \)) and is not related to Arnoldi’s method, whereas the second term \( \|u_N(t) - u^A_{IA}\| = \|u_N(t) - u_{N,N}\| \) can be seen as an error associated with the Arnoldi approximation of the matrix exponential. The following two subsections are devoted to the characterization of these two errors.

4.1. Bound for the truncation error. It will turn out that the truncation error (first term in (4.2)) can be analyzed by relating it to \( \exp(tH_N)e_1 \), i.e., a vector of functions generated by the truncated Hessenberg matrix \( H_N \). Let \( \tilde{e}_N \) denote the difference between the basis functions and the functions generated by the Hessenberg matrix,

\[
   \tilde{e}_N(t) := \tilde{\phi}_N(t) - \exp(tH_N)e_1, \quad \tilde{\phi}_N(t) := \begin{pmatrix} \phi_0(t) \\ \vdots \\ \phi_{N-1}(t) \end{pmatrix}. \tag{4.3}
\]
The following lemma shows that a sufficient condition for the convergence of the first term in (1.2) is that \( \|W_N \tilde{e}_N(s)\| \to 0 \). The following subsections are devoted to the analysis of \( \|W_N \tilde{e}_N(s)\| \) for different basis functions, and in particular lead up the convergence of the truncation error given under general conditions in Theorem 8 and Theorem 11.

**Lemma 7** Let \( u \) be the solution to the ODE (1.1) and \( u_N \) be defined as in (4.1). Suppose the expansion (1.2) is uniformly convergent with respect to \( s \). Then,

\[
\|u(t) - u_N(t)\| \leq \int_0^t \|e^{(t-s)A}\| \|g(s) - W_N e^{sH_N} t\| ds \leq \int_0^t \|e^{(t-s)A}\| ds \left( \max_{\bar{s} \in [0,t]} \|g(\bar{s}) - W_N \bar{\phi}_N(\bar{s})\| + \max_{\bar{s} \in [0,t]} \|W_N \bar{e}_N(\bar{s})\| \right). \tag{4.4}
\]

Moreover, for every \( s \leq t \) we have

\[
\|g(s) - W_N \bar{\phi}_N(\bar{s})\| \to 0 \quad \text{as} \quad N \to \infty. \tag{4.5}
\]

**Proof.** The first bound in (4.4) follows from the variation-of-constants formula

\[
u(t) = e^{tA}u_0 + \int_0^t e^{(t-s)A} g(s) ds,
\]

which gives the exact solution for the ODE (1.1), and from the representation [10, pp. 248]

\[
u_N = [I_n 0] e^{tA} u_N = [I_n 0] \left[ e^{tA} \int_0^t e^{(t-s)A} W_N e^{sH_N} ds \right] e^{tH_N} u_N
\]

\[
eq e^{tA} u_0 + \int_0^t e^{(t-s)A} W_N e^{sH_N} e_1 ds.
\]

The second inequality follows by adding and subtracting \( \bar{\phi}_N(s) \). The limit expression (4.5) follows from the fact that

\[
g(s) - W_N \bar{\phi}_N(s) = \sum_{n=N}^\infty W_n \phi_n(s),
\]

which is the remainder term in the expansion (1.2). The limit vanishes due to the fact that (1.2) is uniformly convergent.

**4.1.1. Bounds on \( \|W_N \tilde{e}_N\| \): scaled monomial basis.** Suppose \( \phi_t \) are scaled monomials such that \( H_N \) is a transposed Jordan matrix, i.e., the truncation of (1.4). The definition of \( \tilde{e}_N \) yields \( \tilde{e}_N(0) = \phi^{(k)}(0) - H_N e_1 \). It follows from the structure (1.4) that, for \( k \leq N, H_N^k e_1 = e_k \) and \( H_N^k e_1 = 0 \) if \( k > N \). Moreover, \( \tilde{e}_N^{(k)}(0) = e_k \) if \( k \leq N \) and \( \tilde{e}_N^{(k)}(0) = 0 \) if \( k > N \). Hence, \( \tilde{e}_N^{(k)}(0) = 0 \) for all \( k \). Since \( \tilde{e}_N \) is analytic and all derivatives vanish, \( \tilde{e}_N(t) = 0 \). Hence, we have obtained the following result.

**Theorem 8** Suppose \( \bar{\phi}_N \) are the scaled monomials, given by \( \phi_t := t^t/\ell! \), and \( H_N \in \mathbb{R}^{N \times N} \) is the leading submatrix of (1.4). Then,

\[
\tilde{e}_N(t) = 0
\]

where \( \tilde{e}_N(t) \) is given by (4.3). Consequently, if the basis functions are the scaled monomials, the truncation error \( \|u(t) - u_N(t)\| \to 0 \) independent of \( t \).
4.1.2. Bounds on $\|W_N \tilde{\varepsilon}_N\|$: Bessel basis functions. If the basis functions are Bessel functions or modified Bessel functions of the first kind, further analysis is required to show that $\|W_N \tilde{\varepsilon}_N\|$ vanishes. The elements of $\tilde{\varepsilon}_N$, denoted by $\varepsilon_{N,k}$, $k = 0, \ldots, N - 1$, can be bounded as follows.

**Lemma 9** Let $H_N \in \mathbb{R}^{N \times N}$ be defined as either (2.4) or (2.6). Then, the vector $\tilde{\varepsilon}_N$ satisfies

$$
\tilde{\varepsilon}_N(t) = \int_0^t e^{(t-s)H_N} J_N(s) e_N \, ds
$$

(4.6)

and is bounded as follows.

(a) For all $t \geq 0$,

$$
\|\tilde{\varepsilon}_N(t)\| \leq \frac{(\frac{1}{2}t)^N}{(N+1)!} \sqrt{2} t e^t.
$$

(4.7)

(b) Suppose $t \geq 2$. Then there exists a constant $\bar{C}(t)$ depending only on $t$ such that for $1 \leq k \leq N$,

$$
|\varepsilon_{N,k}(t)| \leq \bar{C}(t) \frac{t^k}{2^{2N-k} (2N-k+1)!} (N-k)!.
$$

(4.8)

**Proof.** Proof of (4.3): From the properties (2.3) we see that $\tilde{J}_N(t)$ satisfies the initial value problem $	ilde{J}_N(t) = H_N \tilde{J}_N(t) + J_N(t) e_N$, $J(0) = e_1$. Therefore, the error $\tilde{\varepsilon}_N(t) := J_N(t) - e^{tH_N} e_1$ satisfies the initial value problem $\varepsilon_N(t) = H_N \varepsilon_N + J_N(t) e_N$, $\varepsilon_N(0) = 0$, for which the solution is given by (4.4).

The statement (4.7) follows from properties of $H_N$ and Bessel functions as follows. From Lemma 18 we have that $\|e^{(t-s)H_N}\| \leq \sqrt{2} e^{t-s}$ and therefore

$$
\|\tilde{\varepsilon}_N(t)\| \leq \sqrt{2} \int_0^t \|e^{(t-s)H_N}\| \|J_N(s)\| \, ds \leq \sqrt{2} \int_0^t e^{(t-s)} \frac{(\frac{1}{2}t)^N}{N!} e^s \, ds = \frac{(\frac{1}{2}t)^N}{(N+1)!} \sqrt{2} t e^t,
$$

where in the last step we used that for $t > 0$, $|\phi_N(t)| \leq \frac{|\frac{1}{2}t|^N}{N!} e^t$ if $\phi_N = J_N$ or $\phi_N = I_N$, which is a consequence of the formula [24, pp. 49],

$$
|J_n(z)| \leq \frac{|\frac{1}{2}z|^n}{n!} e^{\text{Im}(z)}.
$$

(4.9)

It remains to show (4.8). We first note that, (4.9) and Lemma 18 with $R = t^2$ implies that

$$
|\varepsilon_{N,k}(t)| = \left| \int_0^t e_k^T e^{(t-s)H_N} J_N(s) e_N \, ds \right| \leq \frac{e^t C(t^2)}{t^{2(N-k)} N! 2^{2N-k}} \int_0^t s^N (t-s)^{N-k} \, ds,
$$

(4.10)

where $C(t^2)$ is given by (4.4). We identify the integral on right-hand side of (4.10) as a scaled Beta function $\frac{t^{m+n+1} B(m+1, n+1)}{t^{m+n+1}}$. The conclusion (4.8) now follows from the application of a formula for $B(m+1, n+1)$ in [1] pp. 258. More precisely,

$$
|\varepsilon_{N,k}(t)| \leq \frac{e^t C(t^2)}{t^{2(N-k)} N! 2^{2N-k}} \frac{t^{2k-1} N!(N-k)!}{(2N-k+1)!} = e^t C(t^2) \frac{t^{k+1} N!(N-k)!}{2^{2N-k} (2N-k+1)!}.
$$
We have now derived a bound on $\epsilon_N$ and shown that $\|\epsilon_N(t)\| \to 0$ as $N \to \infty$, when the basis functions are the Bessel functions or the modified Bessel functions of the first kind. Note that this does not necessarily imply that $\|W_N\| \to 0$, since $\|W_N\|_N$ may not be bounded for all $N$. Fortunately, the analyticity of $g(t)$ gives us a bound on the growth of the coefficients $w_k$.

**Lemma 10** Suppose $g$ is analytic in a neighborhood of a disc of radius $t$ centered at the origin. Let $M_t$ be defined as

$$M_t = \max_{|\lambda|=t} |g(\lambda)|.$$  

(4.11)

Let the vectors $w_k$ be the coefficients of the expansion (1.2) of $g(t)$, where the functions $\phi_\ell$ are the Bessel or the modified Bessel functions of the first kind. Then, for $0 \leq t < 2$ we have the bound

$$\|w_k\| \leq M_t k! \left(\frac{2}{t}\right)^k \text{ for all } k \geq 0.$$  

(4.12)

Moreover, for $t \geq 2$, we have the bounds

$$\|w_k\| \leq M_t k! \text{ for all } k \geq 0,$$  

(4.13)

and

$$\|w_k\| \leq M_t k!2^{k} \left(\frac{2}{t}\right)^k \text{ for all } k > \left(\frac{t}{2}\right)^2 + 1.$$  

(4.14)

**Proof.** The closed form (2.16) for the coefficients $w_k$ implies that for all $k \geq 0$

$$\|w_k\| \leq \sum_{\ell=0}^{\left\lfloor \frac{k}{2} \right\rfloor} k(k-\ell-1)! \frac{1}{\ell!} \left(\frac{1}{2\pi i}\int g(\lambda)\lambda^{k-2\ell-1}d\lambda\right).$$  

(4.15)

Combining (4.11) and (4.15) gives us

$$\|w_k\| \leq \frac{M_t}{2} \sum_{\ell=0}^{\left\lfloor \frac{k}{2} \right\rfloor} k(k-\ell-1)! \frac{1}{\ell!} \left(\frac{2}{t}\right)^{k-2\ell}.$$  

(4.16)

Thus, when $t < 2$, we have that for all $k \geq 0$

$$\|w_k\| \leq \frac{M_t}{2} \left(\frac{2}{t}\right)^k \sum_{\ell=0}^{\left\lfloor \frac{k}{2} \right\rfloor} k(k-\ell-1)! \frac{1}{\ell!} \leq \frac{M_t}{2} \left(\frac{2}{t}\right)^k 2k!$$

which gives (4.12). When $t \geq 2$, $(\frac{2}{t})^{k-2\ell} \leq 1$ if $0 \leq \ell \leq \left\lfloor \frac{k}{2} \right\rfloor$, and with a similar reasoning (4.13) follows from (4.11).

In order to show (4.14), we note that (4.16) can be expressed as

$$\|w_k\| \leq \frac{M_t}{2} \sum_{\ell=0}^{\left\lfloor \frac{k}{2} \right\rfloor} c_\ell,$$  

(4.17)
where \( c_0 = k! \left( \frac{1}{t} \right)^k \) and \( c_\ell = \frac{1}{(k-\ell)!} \left( \frac{1}{2} \right)^2 \cdot c_{\ell-1} \) if \( \ell \geq 1 \). When \( 1 \leq \ell \leq \left\lfloor \frac{k}{2} \right\rfloor \), \( (k-\ell)\ell \geq k-1 \), and we see that \( c_\ell \) satisfies \( c_\ell \leq a_k c_{\ell-1} \) such that \( c_\ell \leq a_k^\ell c_0 \), where \( a_k = t^2/4(k-1) \). The conclusion (4.14) follows from (4.17) and the fact that the assumption \( k > 2 \left( \frac{t}{2} \right)^2 + 1 \) implies that \( a_k < 1/2 \) and by taking the limit \( \ell \to \infty \). □

By combining the bound of \( \bar{\varepsilon}_N \) and the bound of \( w_\ell \) we arrive at the following result for \( W_N \bar{\varepsilon}_N(t) \).

**Theorem 11** If \( W_N \) corresponds to the expansion of \( g(t) \) with the Bessel functions or the modified Bessel functions of the first kind, then for all \( t > 0 \)

\[
||W_N \bar{\varepsilon}_N(t)|| \to 0, \quad \text{as} \quad N \to \infty. \tag{4.18}
\]

Consequently, if the basis functions are the Bessel functions or the modified Bessel functions, the truncation error \( ||u(t) - u_N(t)|| \to 0 \) independent of \( t \).

**Proof.** Consider first the case \( 0 \leq t < 2 \). By (4.7) and (4.12) we see that

\[
|| \sum_{\ell=0}^N w_\ell \varepsilon_{N,\ell}(t)|| \leq ||\bar{\varepsilon}_N(t)|| \sum_{k=0}^N ||w_k|| \leq ||\varepsilon_N(t)|| \sum_{k=0}^N \sqrt{2} t M_\ell \left( \frac{2}{\ell} \right)^k \\
\leq \frac{(4/2)^N}{(N+1)!} \sqrt{2} t M_\ell \left( \frac{2}{\ell} \right)^N \left( N! + (N-1)! + \ldots + 1 \right) \\
= \sqrt{2} t M_\ell \left( \frac{1}{N+1} + \frac{1}{(N+1)N} + \ldots + \frac{1}{(N+1)!} \right) \leq \sqrt{2} t M_\ell \left( \frac{2}{N+1} \right).
\]

Consider the case \( t \geq 2 \). Suppose \( N > \tilde{k} := \left\lfloor 2 \left( \frac{t}{2} \right)^2 + 1 \right\rfloor \). We see that

\[
|| \sum_{\ell=0}^N w_\ell \varepsilon_{N,\ell}(t)|| \leq \sum_{\ell=0}^\tilde{k} ||w_\ell|| \varepsilon_{N,\ell}(t) + \sum_{\ell=\tilde{k}+1}^N ||w_\ell|| \varepsilon_{N,\ell}(t). \tag{4.19}
\]

We now show that both of the terms in the right-hand side of (4.19) vanish as \( N \to \infty \). Using the bound (4.13) of Lemma 10 and the bound (4.8) of Lemma 9 with \( k = \ell \), we see that there exists a constant \( \tilde{C}_2(t) := M_\ell \tilde{C}(t)^k \), which are independent of \( N \), such that

\[
\sum_{\ell=0}^\tilde{k} ||w_\ell|| \varepsilon_{N,\ell}(t) \leq \tilde{C}_2(t) \sum_{\ell=0}^\tilde{k} \frac{\ell!(N-\ell)!}{2^{2N-\ell}(2N-\ell+1)!}. \tag{4.20}
\]

Since for \( \ell \leq \tilde{k} \leq N, \ell!(N-\ell)! < (\ell+1)!(N-\ell)! \leq (N+1)! \) and \( 2^{2N-\ell}(2N-\ell+1)! \geq 2^N((N-\tilde{k}) + N + 1)! \), we see that

\[
\frac{(\ell+1)!(N-\ell)!}{2^{2N-\ell}(2N-\ell+1)!} \leq \frac{(N+1)!}{2^N((N-\tilde{k}) + N + 1)!} \leq \frac{1}{2^N N^{N-k}}. \tag{4.21}
\]

By inserting (4.21) into (4.20) we conclude that the first term in (4.19) vanishes as \( N \to \infty \).
For the second term of (4.19), we use the bound (4.12) of Lemma 10 and the bound (4.8), to see that there exists a constant $\tilde{C}_3(t) := M_t \tilde{C}(t)$, which are independent of $N$, such that

$$
\sum_{\ell=k+1}^{N} ||w_{\ell}|| |e_{N,\ell}(t)| \leq C_3(t) \sum_{\ell=k+1}^{N} \left( \frac{2}{\ell} \right) \frac{t^{\ell}}{2(2N-\ell)!} \frac{\ell!(N-\ell)!}{(2N-\ell+1)!} \\
\leq C_3(t) \sum_{\ell=k+1}^{N} \frac{N!}{(2N-\ell+1)!} \\
\leq C_3(t) \left( (N-k-1) \cdot \frac{1}{(N+2)(N+1)} + \frac{1}{N+1} \right),
$$

This implies that the second term in the right-hand side of (4.19) converges to zero as $N \to \infty$ and completes the proof. $\blacksquare$

### 4.2. Error bounds for the Arnoldi approximation.

In order to show convergence of (4.2) we will now study the second term in (4.2). Let

$$
Q_N = \begin{bmatrix}
Q_{1,N+1} \\
Q_{2,N+1}
\end{bmatrix} \in \mathbb{C}^{(n+N+1) \times (N+1)},
$$

where $Q_{1,N} \in \mathbb{C}^{n \times N}$ is the orthonormal matrix and $F_N = Q_N^* A_N Q_N$ the Hessenberg matrix given by the infinite Arnoldi algorithm after $N$ iterations. The Arnoldi relation (3.2), with $B = A_N$, implies that

$$
AQ_{1,N} + WQ_{2,N} = Q_{1,N} F_N + f_{N+1,N} q_{1,N+1} e_N^T \\
H_N Q_{2,N} = Q_{2,N} F_N + f_{N+1,N} q_{2,N+1} e_N^T.
$$

(4.22)

The polynomial approximation property of the Arnoldi method [19] Lemma 3.1] states that for any polynomial $p$ of degree less than $N$ we have $p(A_N) u_N = \beta Q_N p(F_m) e_1$. In our situation we can exploit the structure of $A_N$ when we select $p(z) = z^\ell$. From the second block of $p(A_N) u_N$ we conclude that $H_N e_1 e_1^T = Q_{2,N} F_N e_1$ for all $\ell \leq N - 1$. By stacking this equation as columns into a matrix equation we find that $K_N(H_N, e_1) e_1^{-1} = Q_{2,N} K_N(F_N, e_1)$, such that

$$
Q_{2,N} = K_N(H_N, e_1) K_N(F_N, e_1)^{-1} e_1^{-1},
$$

(4.23)

where $K_N$ denotes the Krylov matrix, defined in (2.7). The orthonormality of $Q_N$ implies that $||Q_N|| = 1$, from which it follows that $||Q_{1,N}|| \leq 1$ and $||Q_{2,N}|| \leq 1$. Consider $A_N$ of the form (1.6) for a general Hessenberg matrix $H_N$. The infinite Arnoldi approximation at step $N$ is given by

$$
[I_n \quad 0] \cdot Q_N \exp(tF_N) e_1 e_1 = Q_{1,N} \exp(tF_N) e_1 e_1 \\
= Q_{2,N} = K_N(H_N, e_1) K_N(F_N, e_1)^{-1} e_1^{-1},
$$

(4.24)

where $\beta = ||u_N||$. We again use the polynomial approximation property, which implies that

$$
\sum_{\ell=0}^{N-1} A_N \beta^\ell = Q_N \sum_{\ell=0}^{N-1} \frac{1}{\ell!} F_N \beta^\ell. \\
\text{Hence, the second term in the error (4.2)}
$$

can be expressed as

$$
u_N(t) - u_N^{(A)}(t) = [I_n \quad 0] \cdot (\exp(tA_N) u_N - Q_N \exp(tF_N) e_1 e_1) = a_N + b_N,
$$

(4.25)
where

\[ a_N := [I_n \ 0] r_N(tA_N)u_N \] (4.26)

\[ b_N := -Q_{1,N}r_N(tF_N)e_1 \beta \] (4.27)

and \( r_N \) denotes the remainder term in the truncated Taylor expansion. We will use an explicit representation of \( r_N \),

\[ r_N(z) = \sum_{\ell=N}^{\infty} \frac{z^\ell}{\ell!} = z^N \varphi_N(z), \] (4.28)

with the standard definition of \( \varphi \)-functions,

\[ \varphi_\ell(z) := \sum_{k=0}^{\infty} \frac{z^k}{(k+\ell)!} = \int_{0}^{1} e^{(1-\tau)z} \frac{\tau^{\ell-1}}{(\ell-1)!} d\tau. \] (4.29)

### 4.2.1. Convergence of \( a_N \) in (4.25)

The analysis of (4.25) is separated into analysis of \( a_N \) and \( b_N \). We first need a reformulation of \( a_N \).

**Lemma 12** Let \( A_N, u_N, r_N \) and \( \varphi_\ell \) be defined as above. Then, the following expression holds

\[ a_N = (tA)^N \varphi_N(tA)u_0 + \sum_{\ell=1}^{N} t^\ell (tA)^{N-\ell} \varphi_N(tA)g^{(\ell-1)}(0) \]

\[ + \sum_{\ell=N+1}^{\infty} t^\ell \varphi_\ell(tA)W_N H_N^{\ell-1} e_1. \] (4.30)

**Proof.** By induction it is readily verified from (1.6) that

\[ A_N^k \begin{bmatrix} u_0 \\ e_1 \end{bmatrix} = \begin{bmatrix} A^k u_0 + \sum_{\ell=1}^{k} A^{k-\ell} W_N H_N^{\ell-1} e_1 \\ e_1 \end{bmatrix}. \]

From this it follows that

\[ [I_n \ 0] r_N(tA_N) \begin{bmatrix} u_0 \\ e_1 \end{bmatrix} = [I_n \ 0] \sum_{k=N}^{\infty} \frac{(tA_N)^k}{k!} \begin{bmatrix} u_0 \\ e_1 \end{bmatrix} \]

\[ = \sum_{k=N}^{\infty} \frac{(tA)^k}{k!} u_0 + \sum_{\ell=1}^{\infty} \sum_{k=N}^{\infty} \frac{t^\ell (tA)^{k-\ell}}{k!} W_N H_N^{\ell-1} e_1 \]

\[ = \sum_{k=N}^{\infty} \frac{(tA)^k}{k!} u_0 + \sum_{\ell=1}^{\infty} \sum_{k=N}^{\infty} \frac{t^\ell (tA)^{k-\ell}}{k!} W_N H_N^{\ell-1} e_1 + \sum_{\ell=N+1}^{\infty} \sum_{k=\ell}^{\infty} \frac{t^\ell (tA)^{k-\ell}}{k!} W_N H_N^{\ell-1} e_1. \] (4.31)

Since \( W_N H_N^{\ell-1} e_1 = g^{(\ell-1)}(0) \) when \( 0 \leq \ell \leq N \), we find for the second term on the last line of (4.31) that

\[ \sum_{\ell=1}^{N} \sum_{k=N}^{\infty} \frac{t^\ell (tA)^{k-\ell}}{k!} W_N H_N^{\ell-1} e_1 = \sum_{\ell=1}^{N} t^\ell (tA)^{N-\ell} \varphi_N(tA)g^{(\ell-1)}(0). \]
For the third term on the last line of (4.31) we see that
\[
\sum_{\ell=N+1}^{\infty} t^{\ell} \frac{(tA)^{k-\ell}}{k!} W_N H_N^{\ell-1} e_1 = \sum_{\ell=N+1}^{\infty} t^{\ell} \varphi_\ell(tA) W_N H_N^{\ell-1} e_1,
\]
from which the claim follows. \( \square \)

We are now ready to state convergence of the first term in (4.25) under general assumptions about the nonlinearity \( g \).

**Theorem 13** Let \( A_N \) be defined as in (1.6). Assume that for the vectors \( g^{(\ell)}(0) \) are bounded by
\[
||g^{(\ell)}(0)|| \leq c ||A||^\ell
\]
for some constant \( c \in \mathbb{R} \). Then, \( a_N \) defined by (4.26) satisfies
\[
a_N \to 0 \quad \text{as} \quad N \to \infty.
\]

**Proof.** We bound the norm of the term (4.30) as
\[
||[I_n 0] \ r_N(tA_N)u_N||_2 \leq \|(tA)^N \varphi_N(tA)u_0\| + \left| \sum_{\ell=1}^{N} t^{\ell} (tA)^{N-\ell} \varphi_N(tA) g^{(\ell-1)}(0) \right|
\]
\[
+ \left| \sum_{\ell=N+1}^{\infty} t^{\ell} \varphi_\ell(tA) W_N H_N^{\ell-1} e_1 \right|.
\]
By Lemma 19 we get a bound for the first term in (4.33) as
\[
\|(tA)^N \varphi_N(tA)u_0\| \leq \frac{|tA|^N \max(1, e^{t|A|})}{N!} ||u_0||.
\]

For the second term in (4.33), we see that
\[
\left| \sum_{\ell=1}^{N} t^{\ell} (tA)^{N-\ell} \varphi_N(tA) g^{(\ell-1)}(0) \right| \leq \sum_{\ell=1}^{N} t^{\ell} ||tA||^{N-\ell} ||g^{(\ell-1)}(0)|| ||\varphi_N(tA)||
\]
\[
\leq \overline{C} \sum_{\ell=1}^{N} ||tA||^{N} \max(1, e^{t|A|}) \frac{N!}{N!} = \overline{C} ||tA||^{N} \max(1, e^{t|A|}) \frac{N!}{(N-1)!},
\]
where \( \overline{C} = C/||tA|| \). Thus, also the second term in (4.33) converges to zero as \( N \to \infty \).

For the third term in (4.33), we use Lemmas 19 and 20 to find that
\[
\left| \sum_{\ell=N+1}^{\infty} t^{\ell} \varphi_\ell(tA) W_N H_N^{\ell-1} e_1 \right| \leq \sum_{\ell=N+1}^{\infty} t^{\ell} ||\varphi_\ell(tA)|| ||G_N|| ||K_N(H_N, e_1)^{-1} H_N^{\ell-1} e_1||
\]
\[
\leq \sum_{\ell=N+1}^{\infty} t^{\ell} \frac{\max(1, e^{t|A|})}{\ell!} ||G_N|| 2\sqrt{N(1+\sqrt{2})}^N
\]
\[
= t^{N+1} \varphi_{N+1}(t) \max(1, e^{t|A|}) 2\sqrt{N(1+\sqrt{2})}^N ||G_N||
\]
\[
\leq t^{N+1} \left( \frac{\max(1, e^{t|A|}) 2\sqrt{N(1+\sqrt{2})}^N ||G_N||}{(N+1)!} \right).
\]
By assumption (4.32),
\[ ||G_N|| \leq ||G_N||_F = \sqrt{\sum_{\ell=0}^{N-1} ||g^{(\ell-1)}(0)||^2} \leq C, \]
\[ \sum_{\ell=0}^{N-1} ||A||^2 \ell! = C \sqrt{\frac{||A||^{2N} - 1}{||A||^2 - 1}}. \]

Thus also the third term in (4.33) converges to zero as \( N \to \infty. \)

4.2.2. Convergence of \( b_N \) in (4.26). Bounding the remainder \( Q_{1,N}r_N(tF_N)e_1 \beta \) in the error expression (4.25) needs in general additional assumptions about \( F_N. \)

Before stating the convergence theorem, we need the following lemma.

**Lemma 14** Assume that \( 1 < ||H_N|| < ||A|| \) and that (4.32) is satisfied for some constant \( c > 0. \) Then, for \( 0 \leq \ell \leq N \)
\[ ||F_N^\ell e_1|| \leq (1 + \beta^{-1}c\ell)||A||^\ell. \]

**Proof.** From (1.6), (2.9) and (4.23) we see that the Hessenberg matrix \( F_N \) is given by
\[ F_N = Q_{1,N}^*A_NQ_N = Q_{1,N}^*AQ_{1,N} + Q_{2,N}^*HNQ_{2,N} + Q_{1,N}^*W_NQ_{2,N} \]
\[ = Q_{1,N}^*AQ_{1,N} + Q_{2,N}^*HNQ_{2,N} + \beta^{-1}Q_{1,N}^*G_NK_N(F_N,e_1)^{-1}, \]
where \( G_N = [g(0), g'(0), \ldots, g^{(N-1)}(0)]. \) Thus, for the norms of the products \( F_N^\ell e_1, 1 \leq \ell \leq N, \) we get the following recursion:
\[ ||F_N^\ell e_1|| \leq ||Q_{1,N}^*AQ_{1,N} + Q_{2,N}^*HNQ_{2,N}||F_N^{\ell-1}e_1|| \]
\[ + \beta^{-1}||Q_{1,N}^*G_NK_N(F_N,e_1)^{-1}F_N^{\ell-1}e_1|| \]
\[ \leq \max(||A||, ||H_N||)||F_N^{\ell-1}e_1|| + \beta^{-1}||Q_{1,N}^*g^{(\ell-1)}(0)|| \]
\[ \leq ||A||^\ell||F_N^{\ell-1}e_1|| + \beta^{-1}c||A||^{\ell-1}, \]

since \( \beta > 1 \) and \( K_N(F_N,e_1)^{-1}F_N^{\ell-1}e_1 = e_\ell \) for \( 1 \leq \ell \leq N. \) By induction we have that
\[ ||F_N^\ell e_1|| \leq ||A||^\ell||F_N^0 e_1|| + \beta^{-1}c \ell||A||^{\ell-1} = ||A||^\ell + \beta^{-1}c \ell||A||^{\ell-1} \leq ||A||^\ell(1 + \beta^{-1}c \ell). \]

We are ready to give the following result, which gives sufficient conditions for the convergence of the Arnoldi error.

**Theorem 15 (Arnoldi error)** Suppose there exists a constant \( c > 0 \) such that (4.32) is satisfied. Suppose Algorithm 7 generates a Hessenberg matrix \( F_N \) such that for some constant \( C, ||F_N^N|| \leq CN^N \) for all \( N > 0. \) Then, \( b_N \) given by (4.27) satisfies
\[ ||b_N|| \to 0 \quad \text{as} \quad N \to \infty. \]

Moreover, the Arnoldi error in (4.25) satisfies
\[ ||u_N(t) - u_N^{1A}(t)|| \to 0 \quad \text{as} \quad N \to \infty. \]

**Proof.** We see from (4.28) that
\[
r_N(tF_N)e_1 = \sum_{\ell=0}^{\infty} \frac{(tF_N)^\ell e_1}{\ell!} = \sum_{k=1}^{\infty} \frac{(tF_N)^k e_1}{(kN + \ell)!} = \sum_{k=1}^{\infty} \frac{(tF_N)^k e_1}{(kN + \ell)!}. \quad (4.34)
\]
We see by Lemma 14 that

\[ \| \sum_{\ell=0}^{N-1} \frac{(tF_N)^\ell e_1}{(kN + \ell)!} \| \leq \sum_{\ell=0}^{N-1} \frac{\|tA\|^\ell}{(kN + \ell)!} \leq \sum_{\ell=0}^{N-1} \frac{\|tA\|^\ell}{(kN + \ell)!} \leq (1 + \beta^{-1} c N) \sum_{\ell=0}^{N-1} \frac{\|tA\|^\ell}{(kN + \ell)!} . \]  

(4.35)

In the last inequality above we use Lemma 19. Thus, we see from (4.34) and (4.35) that

\[ ||b_N|| \leq ||Q_N|| ||r_N(tF_N)e_1|| \beta \leq \sum_{k=1}^\infty \left( \frac{\|tF_N\|^N}{k!} \right) \sum_{\ell=0}^{N-1} \frac{(tF_N)^\ell e_1}{(kN + \ell)!} \beta \leq (\beta + c N) \sum_{k=1}^\infty \frac{e^{\ell \|tA\|}}{(kN)!} \beta \leq (\beta + c N) e^{\|tA\|} \sum_{k=1}^\infty \frac{(tC)^k}{(kN)!} \beta \]

which converges to zero as \( N \to \infty. \)

**Remark 16 (Assumptions in Theorem 15)** Theorem 15 is only applicable when there exists a constant \( C \) such that \( \|F_N\| \leq C N \) for all \( N > 0 \), where \( F_N \) is the Hessenberg matrix generated by Algorithm 1. This is a restriction on the generality of our convergence theory. In our numerical experiments we have seen no indication that the assumption should not be satisfied (see Figure 5.2c). Moreover, the assumption can be motivated by certain intuitive uniformity assumptions and the generic behavior of Arnoldi’s method for eigenvalue problems, as follows. From the definition of the spectral radius, we have

\[ \|F_N\|^{1/\ell} \to \rho(F_N) \quad \text{as} \quad \ell \to \infty. \]  

(4.36)

Moreover, under the condition that the Arnoldi method approximates the largest eigenvalue of \( A_\infty \), we also have

\[ \rho(F_N) \to \rho(A_\infty) \quad \text{as} \quad N \to \infty. \]  

(4.37)

The operator \( \rho(A_\infty) \) is block diagonal and the (1,1)-block is a finite operator \( A \) and the (2,2)-block is a bounded operator (by assumption (1.3b)). Hence, it is natural to assume that \( \rho(A_\infty) = d \in \mathbb{R} \) exists. If \( \rho(A_\infty) \) exists and the limits (4.36) and (4.37) hold also in a uniform sense, we have that \( \|F_N\|^{1/N} \to d \), which implies the assumption.

5. Numerical examples.

5.1. Numerical evaluation of the derivatives \( g^{(\ell)}(0) \). In order to carry out \( N \) steps of the algorithm, we need the expansion coefficients \( w_0, \ldots, w_N \), which are directly available from the derivatives \( g^{(\ell)}(0), \ell = 0, \ldots, N \) via (2.9). If the nonlinearity is not explicit such it is not possible to compute expressions for the derivatives by hand, there are several alternatives. One may use, e.g., symbolic differentiation which is available for several special functions in MATLAB, or the techniques of automatic differentiation can be used [9].

Another alternative is to use matrix functions. If an efficient and numerically stable matrix function implementation of \( h(z) \) is available (see, e.g., [10, Ch. 4]), one
Fig. 5.1: Subfigure (a) shows the absolute error vs. expansion size $N$ for the approximation of $f(t) = \sin^2(t)$ for the three different choices of basis functions. Subfigure (b) and (c) shows the error vs. the Krylov subspace size for the Schrödinger example. (b) $\epsilon = 10^{-5}$, $T = 10$, (c) $\epsilon = 10^{-3}$, $T = 0.5$.

may use the fact that

$$h(H) e_1 = \begin{bmatrix} h(0) \\ h'(0) \\ h''(0)/2 \\ \vdots \\ h^{(N-1)}(0)/N! \end{bmatrix}$$

for $H = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & \cdots & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & \cdots & 1 & 0 \end{bmatrix} \in \mathbb{R}^{N \times N}$.

Also, there exists methods to compute derivatives by numerically integrating the contour integral in the Cauchy integral formula \[4\].

5.2. 1-D Schrödinger equation with inhomogeneity. We first consider a finite difference spatial discretization (with 100 points) of the initial value problem

$$i \partial_t u = -\epsilon \partial_{xx} u + f(t) \sin(2^4 \pi x (1 - x)), \quad x \in [0, 1], \quad t \in [0, T] \quad (5.1)$$

subject to periodic boundary conditions, with $f(t) = (1 + i) \sin(t)^2$ and initial condition $u(x, 0) = \exp(-100(x - 0.5)^2)$. Figure 5.1a depicts the absolute error of the approximation $f(t) \approx W_N \exp(tH_N) e_1 = \sum_{\ell=0}^{N-1} w_\ell \phi_\ell^{(N)}(t)$, for the three different choices of $W_N$ and $H_N$, for $1 \leq N \leq 50$ and $t = 6$. We again compare the infinite Arnoldi algorithm approximation of $u(T)$ for the three different expansion of $f(t)$. In Figures 5.1a we illustrate the relative 2-norm error of the approximations vs. the Krylov subspace size, when $\epsilon = 10^{-5}$ and $\epsilon = 10^{-3}$. In Fig. 5.1b we observe different truncation errors for different basis functions. Analogously, a difference in convergence speed of Alg. 1 can be observed in Fig. 5.1b.

In a sense, the convergence of the linear part (associated with $A$) dominates the total error in the case of the strong linear part ($\epsilon = 10^{-3}$), and therefore the choice of basis does not affect the convergence, which is also observed in Fig. 5.1b.

We illustrate the competitiveness of the approach in terms of CPU-time$^2$ in Figures 5.2, when $\epsilon = 10^{-5}$ and $\epsilon = 10^{-3}$. We use three different integrators: the infinite

$^1$All experiments are carried out on a desktop computer with a 2.90 GHz single Pentium processor using MATLAB.

20
Arnoldi algorithm with the Bessel functions of the first kind and the MATLAB implementations of the Runge-Kutta method ode45 and ode15s.

Note that the Matlab integrators use adaptive time-stepping, and that the infinite Arnoldi method performs a single time step for which the subspace size is set a priori. When \( \epsilon = 10^{-5} \), ode45 needed 10,16,25,40,86 time steps to obtain the results of Figure 5.2 and ode15s 10,13,51,96,189, respectively. When \( \epsilon = 10^{-3} \), ode45 needed 29,30,31,33,33 time steps, and ode15s 10,15,22,60,124 time steps.

When the linear part is not very stiff, we see that the explicit integrator ode45 gives better results than the stiff implicit solver ode23. For this particular simulation setup, the infinite Arnoldi method is faster than the MATLAB Runge-Kutta implementations, as can be observed in Figures 5.2.

Figure 5.2c gives a numerical justification for the assumptions used in the error analysis given in Section 4.2.2. We consider the numerical example above with the parameter \( \epsilon = 10^{-3} \). We observe that up to machine precision, \( \frac{||F_N||^{1/N}}{\rho(A)} \to \frac{1}{1} \) as \( N \to \infty \), such that the conditions discussed in Remark 16 appear to be satisfied.

Fig. 5.2: Subfigures (a) and (b) show the error vs. CPU time in seconds for the 1-D Schrödinger example, with (a) \( \epsilon = 10^{-5} \), \( T = 10 \), and (b) \( \epsilon = 10^{-3} \), \( T = 0.5 \). Subfigure (c) show the indicator \( \frac{||F_N||^{1/N}}{\rho(A)} - 1 \)

5.3. 2-D Schrödinger equation with inhomogeneity. In order to illustrate generality of the infinite Arnoldi method, we consider a finite difference spatial discretization (with 100^2 points) of the two-dimensional initial value problem

\[
\begin{align*}
    i\partial_t u &= -\epsilon(\partial_{xx} u + \partial_{yy} u) + f(t) \sin(2^4 \pi x(1-x) y(1-y)), & x \in [0,1], & t \in [0,T] \\
    u(x,0) &= \exp(-100((x-0.5)^2 + (y-0.5)^2))
\end{align*}
\]  

subject to periodic boundary conditions, with \( f(t) \) as in (5.1) and initial condition \( u(x,0) = \exp(-100((x-0.5)^2 + (y-0.5)^2)) \).

We compare the infinite Arnoldi algorithm approximation of \( u(T) \) for the three different expansion of \( f(t) \). Figures 5.3 depict the relative 2-norm error of the approximations vs. the Krylov subspace size, when \( \epsilon = 5 \cdot 10^{-3} \) and \( \epsilon = 5 \cdot 10^{-2} \). We see again that the convergence of the linear part starts to dominate the total error as the linear part gets larger.

Figures 5.4 depict the relative 2-norm errors of the approximations of \( u(t) \) vs. the CPU time when \( \epsilon = 5 \cdot 10^{-2} \) and \( \epsilon = 5 \cdot 10^{-3} \), for the three different integrators: infinite Arnoldi with Bessel expansion and Matlab codes ode45 and ode15s.
Fig. 5.3: Error vs. the Krylov subspace size for the Schrödinger example. Left: $\epsilon = 5 \cdot 10^{-3}, T = 10$, right: $\epsilon = 5 \cdot 10^{-2}, T = 0.25$.

Fig. 5.4: Error vs. CPU time in seconds for the 2-D Schrödinger example. Left: $\epsilon = 5 \cdot 10^{-3}, T = 10$, right: $\epsilon = 5 \cdot 10^{-2}, T = 0.25$.

6. Concluding remarks and outlook. The main contribution of this paper is a new algorithm for inhomogeneous linear ODEs and the associated convergence theory. The algorithm belongs to a class of methods exponential integrators. Many of the techniques that are combined with exponential integrators are likely feasible in this situation. For instance, a potentially faster approach can be derived by repeating the algorithm for different $t$, i.e., instead of integrating to $t = T$ directly, the algorithm can be applied for $h_1, \ldots, h_m$ where $T = h_1 + \cdots + h_m$. Moreover, it seems also feasible to apply the algorithm to certain nonlinear equations, by simple linearization procedure, although it would certainly not be efficient for all nonlinear problems. See [4] for variants of exponential integrators.

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REFERENCES

[1] M. Abramowitz and I. A. Stegun, editors. Handbook of mathematical functions with formulas, graphs and mathematical tables, volume 55 of Applied Mathematics Series. National Bureau of Standards, 1964.
[2] A. H. Al-Mohy and N. J. Higham. Computing the action of the matrix exponential, with an application to exponential integrators. SIAM J. Sci. Comput., 33:488–511, 2011.
[3] M. Benzi and N. Razouk. Decay bounds and $O(n)$ algorithms for approximating functions of sparse matrices. ETNA, Electron. Trans. Numer. Anal., 28:16–39, 2007.
we know that eigendecomposition is the colleague matrix of the Chebyshev polynomial $T$ and if $H$ moreover, $\alpha$ where $\kappa$ decomposition of $H$ eigenvector matrix in 2-norm, i.e., $\kappa_N$.

Lemma 17 Let $H_N \in \mathbb{R}^{N \times N}$ be defined as in (2.4) or as in (2.5), and let the eigendecomposition of $H_N$ be given as $H_N = VAV^{-1}$. Then, the condition number of the eigenvector matrix in 2-norm, i.e., $\kappa_2(V) = ||V|| ||V^{-1}||$, is given by $\kappa_2(V) = \sqrt{\nu}$.

Moreover, $||e^{tH_N}|| \leq \sqrt{\nu} e^{\alpha(H_N)}$, (A.1)

where $\alpha(A)$ denotes the spectral abscissa of $A$. If $H_N$ is given by (2.4), $\alpha(H_N) = 0$ and if $H_N$ is given by (2.6) we have that $\alpha(H_N) \leq 1$.

Proof. We first consider the case where $H_N$ is defined by (2.4). Note that $H_N$ is the colleague matrix of the Chebyshev polynomial $T_N(x)$ [22 Theorem 18.1], and we know that $H_N$ has $N$ different eigenpairs $(\lambda, \nu)$ where $\lambda$-values are the zeros of $T_N(x)$, and $\nu$-vectors are of the form $\nu = [T_0(\lambda) \quad \ldots \quad T_{N-1}(\lambda)]^T$. Thus, $H_N$ has the eigendecomposition $H_N = VAV^{-1}$, where $V = \begin{bmatrix} T_0(t_0) & \ldots & T_0(t_{N-1}) \\ \vdots & \ddots & \vdots \\ T_{N-1}(t_0) & \ldots & T_{N-1}(t_{N-1}) \end{bmatrix}$.
and \((t_0, \ldots, t_{N-1})\) are the \(N\) different zeros of \(T_N(\cdot)\). The Chebyshev polynomials satisfy a discrete orthogonality condition

\[
\sum_{k=0}^{N-1} T_i(t_k) T_j(t_k) = \begin{cases} 
0 & , \ i \neq j \\
N & , \ i = j = 0 \\
N/2 & , \ i \neq j.
\end{cases}
\] (A.2)

With (A.2) we verify that \(VV^*\) is a diagonal matrix where all elements are equal to \(N/2\) except the first element which is equal to \(N\). Hence, \(R\)-matrix in the QR-decomposition of \(V^* = QR\) is a diagonal matrix and we conclude that there exists \(Q \in \mathbb{R}^{n \times n}\) such that \(QQ^* = Q^*Q = I\) and \(V = \alpha \text{diag}(\sqrt{2}, 1, \ldots, 1)Q^*,\) where \(\alpha = \sqrt{N/2}\). We see that \(||V|| = |\alpha| \sqrt{2}\) and \(||V^{-1}|| = 1/|\alpha|.\) Therefore \(\kappa_2(V) = \sqrt{2}\).

Let now \(H_N\) be defined as in (2.4). Define the polynomials \(\tilde{T}_n(x), n \geq 0\) as \(\tilde{T}_n(x) = i^n T_n(-ix)\), where \(T_n\) is the \(n\)th Chebyshev polynomial. We now use the recurrence relation of Chebyshev polynomials; see, e.g., [22, Chapter 3]. We see that \(\tilde{T}_i\) satisfies \(\tilde{T}_0(x) = 1, \tilde{T}_1(x) = x\) and \(T_{n+1}(x) = -2x T_n(x) + T_{n-1}(x)\). Therefore, the eigenvalues of \(H_N\) are the zeros of the polynomial \(\tilde{T}_n(x)\), which are \(i\) multiplied with the zeros of the polynomial \(T_n(x)\). The corresponding eigenvectors are of the form \(v = \left[\tilde{T}_0(\lambda) \quad \cdots \quad \tilde{T}_{n-1}(\lambda)\right]^T\). From the condition (A.2) it follows that the polynomials \(\tilde{T}_i(x)\) satisfy the condition

\[
\sum_{k=0}^{N-1} \tilde{T}_i(t_k) \tilde{T}_j(t_k) = \begin{cases} 
0 & , \ i \neq j \\
N & , \ i = j = 0 \\
i^j N/2 & , \ i \neq j
\end{cases}
\] (A.3)

and the rest of the proof follows as for the modified Bessel functions. The bound (A.1) follows from the fact that \(||e^{tH_N}\|| = ||Ve^{tV}V^{-1}|| \leq \kappa(V) ||e^{tH}||\). The conclusion about the spectral abscissa if \(H_N\) is given by (2.4) follows from Gershgorin’s theorem and the conclusion of if \(H_N\) is given by (2.4) follows from the fact that the eigenvalues of \(H_N\) are imaginary.

**Lemma 18** Let \(H_N\) be defined either as (2.4) or (2.6) and let \(t > 0\). Let \(R \in \mathbb{R}\) be any value such that \(R > t\). Then, the elements of \(e^{tH_N}\) are bounded as

\[
(e^{tH_N})_{i,j} \leq C(R) \lambda^{|i-j|},
\] (A.3)

where \(\lambda = \frac{t}{\pi}\) and

\[
C(R) = \max(|| \exp(tH_N)||, 2\sqrt{2} e^{R+\frac{\pi t}{\pi}} (1-\lambda)).
\] (A.4)

**Proof.** We may apply directly the bound (3.10) in [3, Sec. 3.7]. We know that \(tH_N\) has its spectrum inside the interval \([-t,t]\), which has the logarithmic capacity \(\rho = t/2\). For the integration contour we take the same ellipse as in [3], so \(V = 2\pi\) and \(M(R) = e^{R+\frac{\pi t}{\pi}}\), where \(R > t\) can be chosen freely. Let \(H_N = VDV^{-1}\) be the diagonalization of \(H_N\). From Lemma 17 we know that \(\kappa(V) = \sqrt{2}\). The bound (3.10) of [3] gives (A.3).

\section{Conclusion}

...
Lemma 19  For any matrix $A \in \mathbb{C}^{n \times n}$ and positive integer $\ell$,

$$||\varphi(A)|| \leq \frac{\max(1, e^{\mu(A)})}{\ell!},$$

where $\mu(A)$ denotes the logarithmic norm, i.e., $\mu(A) = \max\{\lambda : \lambda \in \Lambda(A)\}$.

Proof. From (1.20) we see that

$$||\varphi(A)|| = \int_0^1 e^{(1-t)A} \frac{t^{\ell-1}}{(\ell-1)!} dt \leq \int_0^1 \|e^{(1-t)A}\| \frac{t^{\ell-1}}{(\ell-1)!} dt.$$

Using the Dahlquist bound $\|e^A\| \leq e^{\mu(A)}$ and the fact that $\mu((1-t)A) \leq \max\{0, \mu(A)\}$ for $0 \leq t \leq 1$, the claim follows. \hfill \square

Lemma 20  Let $H_N$ be defined as in (2.3) or (2.6). Then, for $k \geq N$,

$$||K_N(H_N, e_1)^{-1}H_N^k e_1|| \leq 2\sqrt{N}(1 + \sqrt{2})^N.$$

Proof. Let $p_N(\lambda) = \sum_{t=0}^N \alpha_t \lambda^t$ be the characteristic polynomial of $H_N$. Define

$$\widetilde{\alpha}_N = \begin{bmatrix} \alpha_0 \\ \vdots \\ \alpha_{N-1} \end{bmatrix}, \quad \text{and} \quad C(\widetilde{\alpha}_N) = \begin{bmatrix} 1 & \widetilde{\alpha}_N \\ & \ddots & \ddots \\ & & & 1 \end{bmatrix} \in \mathbb{R}^{N \times N}.$$

Suppose $k \geq N$. Since $H_N^k e_1 = -\sum_{t=0}^{N-1} \alpha_t H_N^t e_1 = K_N(H_N, e_1)\widetilde{\alpha}_N$, we see that

$$H_NK_N(H_N, e_1) = [H_N e_1 \ldots H_N^N e_1] = K_N(H_N, e_1)C(\widetilde{\alpha}_N),$$

and since $H_N^{N-1} e_1 = K_N(H_N, e_1) e_N$, we see that

$$H_N^k e_1 = H_N^{k-N+1}K_N(H_N, e_1)e_N = K_N(H_N, e_1)C(\widetilde{\alpha}_N)^{k-N+1}e_N,$$

i.e.,

$$K_N(H_N, e_1)^{-1}H_N^k e_1 = C(\widetilde{\alpha}_N)^{k-N+1}e_N.$$  

(A.6)

We recognize that $C(\widetilde{\alpha}_N)$ is the companion matrix of the $N$th Chebyshev polynomial $T_N$, and that $V_N e_i = e_i \Lambda_N$, where $\lambda_1, \ldots, \lambda_N$ are the zeroes of $T_N$, $\Lambda_N = \text{diag}(\lambda_1, \ldots, \lambda_N)$ and $V_N$ is the Vandermonde matrix corresponding to $\lambda_1, \ldots, \lambda_N$, i.e.,

$$V_N = \begin{bmatrix} 1 & \lambda_1 & \ldots & \lambda_1^{N-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \lambda_N & \ldots & \lambda_N^{N-1} \end{bmatrix}. $$

Thus for $\ell \geq 1$, $C(\widetilde{\alpha}_N)^\ell = V_N^{-1} A_N^\ell V_N$, and subsequently for any matrix norm $|| \cdot ||^*$

$$||C(\widetilde{\alpha}_N)^\ell||^* \leq ||V_N^{-1}||^* ||A_N^\ell||^* ||V_N|| \leq ||V_N^{-1}||^* ||V_N||,$$

for all $\ell \geq 1$, \hfill (A.7)

since $|\lambda_i| \leq 1$ for all $1 \leq i \leq N$. From [7] Thm. 4.3 and Example 6.2, we know that

$$||V_N^{-1}||^* ||V_N|| \leq 2(1 + \sqrt{2})^N.$$

(A.8)

Thus, using (A.6), we see that for $k \geq N$ $||K_N(H_N, e_1)^{-1}H_N^k e_1|| \leq ||C(\widetilde{\alpha}_N)^{k-N+1}|| \leq \sqrt{N} ||C(\widetilde{\alpha}_N)^{k-N+1}||^*$ and the statement follows from (A.7) and (A.8). \hfill \square