Computing the reciprocal of a φ-function by rational approximation

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Abstract
In this paper, we introduce a family of rational approximations of the reciprocal of a φ-function involved in the explicit solutions of certain linear differential equations, as well as in integration schemes evolving on manifolds. The derivation and properties of this family of approximations applied to scalar and matrix arguments are presented. Moreover, we show that the matrix functions computed by these approximations exhibit decaying properties comparable to the best existing theoretical bounds. Numerical examples highlight the benefits of the proposed rational approximations w.r.t. the classical Taylor polynomials and other rational functions.

Keywords Matrix functions · Rational approximation · Structured matrices

Mathematics Subject Classification (2010) MSC 65F60

1 Introduction
Numerical methods for the computation of matrix functions have witnessed growing interest in recent years (see [18, 20] and the references given therein). One important
class of applications is the solution of some classical problems for ordinary or partial differential equations. Several methods have been developed for the evaluation of the matrix \( \phi \)-functions \( \phi_k(A) \), \( k \geq 0 \), where \( A \) is a large and possibly sparse matrix, and \( \phi_k(z) \) are entire functions defined recursively by \( \phi_{k+1}(z) = \frac{1}{z} \phi_k(z) - \frac{1}{k!} \) with \( \phi_0(z) = e^z \) [21].

Here we focus on the related issue of approximating the matrix function \( \psi_1(A) \) where \( \psi_1(z) \) is a meromorphic function defined as the reciprocal of \( \phi_1(z) \), that is,

\[
\psi_1(z) = \phi_1(z)^{-1} = \frac{z}{e^z - 1}
\]

and \( A \) is banded or more generally rank-structured (see [13] for a survey on such matrices). This problem also plays an important role in a number of applications. We describe two of these applications in more detail.

1.1 Applications

Two-point inverse problems for first-order differential equations are frequently encountered in mathematical physics (see Chapter 7 in [27]). As a model, in this paper we consider the differential problem

\[
\frac{du}{dt} = Au(t) + p, \quad 0 \leq t \leq \tau, \quad (1.1)
\]

where \( A \in \mathbb{R}^{d \times d} \) is given, while \( p \in \mathbb{R}^d \) is unknown. In order to find the solution \( u : [0, \tau] \to \mathbb{R}^d \) of (1.1) and the vector \( p \) simultaneously, the overdetermined conditions

\[
u(0) = u_0 = g, \quad u(\tau) = h, \quad (1.2)
\]

can be imposed. Note that a more general formulation of the inverse problem (1.1), (1.2) in a Banach space with a closed linear operator \( A \) is treated in [30, 31], whereas a new formula for the solution of the problem (1.1), (1.2) using Bernoulli polynomials is given in [14].

Now assume that the complex numbers

\[
2\pi ik/\tau, \quad k = \pm 1, \pm 2, \ldots
\]

(1.3)
do not belong to the spectrum of \( A \). Define the complex-valued functions

\[
q_t(z) = \frac{z}{e^{t_z} - 1} e^{zt}, \quad w_t(z) = \frac{e^{zt} - 1}{e^{t_z} - 1}, \quad 0 \leq t \leq \tau, \quad z \in \mathbb{C} \quad (1.4)
\]

with \( q_t(0) = \frac{1}{t \tau}, \quad w_t(0) = \frac{t}{\tau} \). The complex functions \( q_t(z), w_t(z) \) are meromorphic in \( z \) with poles (1.3). One can check directly that the solution of the inverse problem (1.1), (1.2) is given by the formulas

\[
p = q_0(A)(h - g) - Ag \quad (1.5)
\]

and

\[
u(t) = w_t(A)(h - g) + g, \quad 0 \leq t \leq \tau. \quad (1.6)
\]
Using (1.5) and the formula $$q_0(z) = \psi_1(\tau z)/\tau$$ we obtain the formula

$$p = \frac{1}{\tau} \psi_1(\tau A) (h - g) - Ag. \quad (1.7)$$

to compute the unknown vector $$p$$ via the function $$\psi_1$$.

Notice also that the formula

$$v(t) = q_t(A)v_0, \quad 0 \leq t \leq \tau$$

yields the solution of the nonlocal problem

$$\frac{dv}{dt} = Av(t), \quad 0 \leq t \leq \tau, \quad \int_0^\tau v(t) \, dt = v_0 \quad (1.8)$$

studied by the authors in [7].

Computing the inverse of $$\phi_1(A)$$, with $$A \in \mathbb{R}^{d \times d}$$, is also a fundamental task in the application of exponential integrators for the numerical solution of systems of differential equations. The reason is twofold. First, certain integration schemes called Runge-Kutta Munthe-Kaas (RKMK) methods [22, 25, 26] for computing numerical solutions of differential equations that are guaranteed to evolve on a prescribed manifold require explicitly the approximation of the function $$\psi_1$$ applied to a matrix. More precisely, suppose that $$G$$ is a finite-dimensional Lie group acting transitively on a smooth manifold $$M$$. In many classical examples, $$M = G$$ is a matrix Lie group, acting on itself by left or right multiplication. Denote by $$\mathfrak{g}$$ the Lie algebra of $$G$$ and let $$p$$ be a fixed base point in $$M$$. Any smooth curve $$y(t)$$ on $$M$$ in a neighborhood of $$p$$ can be seen as the image of a curve $$\sigma(t)$$ through the origin of $$\mathfrak{g}$$ via the exponential mapping:

$$y(t) = \exp(\sigma(t)) \cdot p, \quad \sigma(0) = 0.$$  

A differential equation for $$y(t)$$ on the manifold takes the form $$\frac{d}{dt} y = F(y)$$, where $$F$$ is a vector field on $$M$$, and it can be reformulated as a differential equation for $$\sigma(t)$$:

$$\frac{d}{dt} \sigma(t) = d\exp_{\sigma}^{-1}(f(\exp(\sigma) \cdot p)),$$

where $$f : M \longrightarrow \mathfrak{g}$$ is a suitable representation of the vector field $$F$$ (see, e.g., [25] or [8] for details). This equation holds on a linear space, where one may apply a standard Runge-Kutta method. A crucial step in doing so is the evaluation of the reciprocal of the differential of the exponential map:

$$d\exp_{\sigma}^{-1}(v) = \frac{z}{\exp(z) - 1} \bigg|_{z = \text{ad}_\sigma v},$$

where $$\text{ad}_\sigma$$ denotes the commutator: $$\text{ad}_\sigma (v) = [\sigma, v]$$. In other words, in the matrix manifold case each RKMK step requires the computation of $$\psi_1([M, N])$$, where $$M \in \mathbb{R}^{d \times d}$$ is fixed and $$[M, N] = MN - NM$$ is the matrix commutator. Including the evaluation of the map $$\psi_1([M, N])$$ in numerical algorithms seems to be awkward and several polynomial approximations of $$\psi_1(z)$$ have been presented in the related literature (compare with [8] and the references given therein).

As a second remark on the role of approximating $$\psi_1(A)$$ in the context of exponential integrators, we observe that the study of reliable procedures for the
evaluation of $\psi_1(A)$ and $\psi_1(A)v$ based on rational approximations of the meromorphic function $\psi_1(z)$ might be used to foster the development of rational Krylov methods for computing $\phi_1(A)$ and $\phi_1(A)v$, which is the main computational bulk in exponential integrators for stiff systems of differential equations [16]. Indeed the properties of these methods depend heavily on the features of the underlying rational approximations for the selection of the poles and of the subspace of approximation.

1.2 Approximation of $\psi_1(A)$

Customary approximations of $\psi_1(A)$ derived from truncated Taylor expansions go back to the work of Magnus [23]. These approximations are quite accurate if the norm of the matrix $A$ is sufficiently small. On the other hand, rational functions may exhibit approximation properties and convergence domains superior to polynomials provided that the poles of the rational functions involved have been chosen in a suitable way. Moreover, if $A$ is banded or even just rank-structured then the same property holds in a certain approximate sense for the matrix $\phi_1(A)$ and thus a fortiori for its inverse $\psi_1(A)$. Polynomial approximations for the function $\psi_1(z)$ often require a quite high degree of the approximating polynomial in order to achieve a reasonable quality of approximation of the numerical rank structure and the decaying properties of the matrix $\psi_1(A)$. Rational approximations would typically obtain the same quality with substantially fewer degrees of freedom.

In this paper we present new algorithms that efficiently approximate the functions of a matrix argument involved in the solution of (1.1), (1.2). In particular, we propose a novel family of fixed-poles mixed polynomial-rational approximations of $\psi_1(z)$ required for the computation of the vector $p$ according to (1.7). By combining Fourier analysis methods applied to the function $q_t(z)/z$ with classical tools for Fourier series acceleration [12] for any fixed $s > 1$ and $m \geq s$ we obtain approximations of $\psi_1(A) = (\phi_1(A))^{-1}$ of the form

$$\psi_1(A) \simeq p_s(A) + \sum_{k=1}^{m} \gamma_{k,s} A^{\tau_s} (A^2 + k^2 I_d)^{-1},$$

where $p_s(z)$ is a polynomial of degree $\ell = \ell(s)$ and $\tau_s = \tau(s) \in \mathbb{N}$. These novel expansions compare favorably with polynomial approximations based on the Maclaurin series as well as other rational Padé approximants determined by inverting the approximation of $\phi_1(A)$. Specifically:

1. Theory and numerical evidence show that the formulas (1.9) are accurate on larger domains than their polynomial counterparts thus allowing for larger steps in integration schemes.
2. Typically rational approximations based on (1.9) and Padé techniques behave similarly. However, the computation $\psi_1(A)$ and $\psi_1(A)v$ by means of (1.9) is insensitive of numerical difficulties due to the conditioning of $\phi_1(A)$. Also, computations based on (1.9) are inherently parallelizable.
3. Besides this, the scheme (1.9) can be applied easily and efficiently to remarkable classes of matrices including band, rank structured and displacement structured...
matrices, which are often found in applications (e.g., from discretization of differential operators). Indeed, fast and robust inversion algorithms are available for these classes of matrices, together with cheap storage techniques. In particular, when $A$ is rank-structured the action of the matrix $\psi_1(A)$ on a vector can be computed efficiently using the direct fast solver for shifted linear systems proposed in [7].

4. For a symmetric banded matrix $A$ these novel approximations (1.9) yield a computable reconstruction of the associated matrix function $\psi_1(A)$ which exhibits decaying properties comparable to the best existing theoretical bounds and significantly superior to the behavior of the corresponding polynomial approximations. The matrix function $\psi_1(A)$ can thus be manipulated efficiently using its resulting data-sparse format combined with the rank-structured matrix technology [13].

5. Note that the rational part of (1.9) has poles $\{\pm ik\}_{k=1,...,m}$. The choice of a fixed set of poles can be advantageous in view of application to rational Krylov methods for computing $\psi_1(A)$ or $\psi_1(A)v$, as well as for error analysis.

1.3 Structure of the paper

The paper is organized as follows. In Section 2 we present a general scheme for the design of accurate rational approximations of the matrix functions involved in the solution of (1.1), (1.2). In Section 2.1 this scheme is specialized for the construction of mixed polynomial-rational approximations of the meromorphic function $\psi_1(z)$. An application to a multi-degree of freedom physical system is illustrated in Section 3. In Section 4 we investigate both theoretical and computational properties of the application of mixed polynomial-rational formulas to computing $\psi_1(A)$ where $A$ is a symmetric banded matrix. Finally, conclusions and future work are presented in Section 5.

2 Rational approximation of the inverse problem and the reciprocal of the $\phi_1$-function

The solvability of the inverse problem (1.1), (1.2) in an abstract Banach space is studied in [14, 30, 31]. Under the assumption that all the numbers (1.3) are regular points of the linear operator $A$, the inverse problem (1.1), (1.2) has a unique solution. Without loss of generality one can assume that $\tau = 2\pi$. As it was mentioned above in the matrix case this solution is given by the formulas (1.4), (1.5), (1.6).

We introduce the auxiliary function

$$r_t(z) = \frac{e^{zt}}{e^{z2\pi} - 1}, \quad 0 \leq t \leq 2\pi. \quad(2.10)$$

Using the formulas (1.4) we have

$$q_t(z) = zr_t(z), \quad w_t(z) = r_t(z) - r_0(z), \quad 0 \leq t \leq 2\pi. \quad (2.11)$$
Expanding the function \( r_t(z) \) in the Fourier series of \( t \) we obtain
\[
r_t(z) = \frac{1}{2\pi} \left( \frac{1}{z} + \sum_{k \in \mathbb{Z} / \{0\}} \frac{e^{ikt}}{z - ik} \right), \quad 0 < t < 2\pi.
\]

We consider the equivalent representation with the real series given by
\[
r_t(z) = \frac{1}{2\pi z} + \frac{1}{\pi} \sum_{k=1}^{\infty} (z \cos(kt) - k \sin(kt))(z^2 + k^2)^{-1}, \quad 0 < t < 2\pi. \tag{2.12}
\]

It is well known that the convergence of this series must depend strongly on the smoothness of the periodic extension of \( r_t(z) \). Acceleration techniques proposed in [12] make use of the Bernoulli polynomials for the approximate reconstruction of jumps.

Applying the formula
\[
\frac{1}{z^2 + k^2} = \frac{1}{k^2} - \frac{z^2}{k^2(z^2 + k^2)}
\]

(2.13) to the last entry in (2.12) we obtain that for \( 0 < t < 2\pi \) it holds
\[
r_t(z) = \frac{1}{2\pi z} + \frac{1}{\pi} \sum_{k=1}^{\infty} (z \cos(kt) + \frac{1}{k} z^2 \sin(kt))(z^2 + k^2)^{-1} - \frac{1}{\pi} \sum_{k=1}^{\infty} \frac{1}{k} \sin(kt).
\]

Since
\[
2 \sum_{k=1}^{\infty} \frac{1}{k} \sin kt = \pi - t, \quad 0 < t < 2\pi
\]

we arrive at the following formula for \( 0 < t < 2\pi \),
\[
r_t(z) = \frac{1}{2\pi z} + \frac{t - \pi}{2\pi} + y_t(z) \tag{2.14}
\]

with
\[
y_t(z) = \frac{1}{\pi} \sum_{k=1}^{\infty} (z \cos(kt) + \frac{1}{k} z^2 \sin(kt))(z^2 + k^2)^{-1}. \tag{2.15}
\]

If \( z \in K \subset \mathbb{C}, K \) compact set, then definitively we have
\[
|z - ik|^{-1} \leq \frac{C}{|k|}, \tag{2.16}
\]

and, therefore, using the Weierstrass M-test one can easily check that the series in (2.14) converges uniformly in \((t, z) \in [0, 2\pi] \times K\). Hence, by continuity we may extend the formula (2.15) over the whole interval \([0, 2\pi]\).

Combining the formulas (1.4) and (2.14) we get
\[
q_t(z) = \frac{1}{2\pi} + z \frac{t - \pi}{2\pi} + z y_t(z) \tag{2.17}
\]

and
\[
w_t(z) = \frac{t}{2\pi} + (y_t(z) - y_0(z)). \tag{2.18}
\]
Here there are no singularities at \( z = 0 \). Inserting (2.17), (2.18) in (1.5), (1.6) we obtain the formulas for the solution of the inverse problems

\[
p = \left( \frac{1}{2\pi} I - \frac{1}{2} A + Ay_0(A) \right) (h - g) - Ag
\]  

(2.19)

and

\[
u(t) = \left( \frac{t}{2\pi} I + (y_t(A) - y_0(A)) \right) (h - g) + g, \quad 0 \leq t \leq 2\pi
\]  

(2.20)

with

\[
y_t(A) = \frac{1}{\pi} \sum_{k=1}^{\infty} \left( A \cos(kt) + \frac{1}{k} A^2 \sin(kt) \right) \left( A^2 + k^2 I \right)^{-1}.
\]  

(2.21)

The rate of convergence of the series in (2.21) is the same as for the series \( \sum_{k=1}^{\infty} k^{-2} \). It can be improved by using repeatedly the equality (2.13) as above. For each integer \( k \geq 0 \) denote as \( B_k(t) \) the Bernoulli polynomials (extended by periodicity onto the real line) defined by

\[
\frac{ze^{zt}}{e^z - 1} = \sum_{k=0}^{+\infty} \frac{B_k(t)}{k!} z^k, \quad |t| < 2\pi,
\]  

(2.22)

\[
B_k = B_k(0), \quad k \geq 0,
\]

where \( B_k \) are the Bernoulli numbers. Then, using (2.13) we prove by induction the following formulas.

**Lemma 1** Let \( t \in [0, 2\pi] \) and \( y_t(z) : \mathbb{C} \to \mathbb{C} \) be defined as in (2.15). Then we have

\[
y_t(z) = p_{n,t}(z) + s_{n,t}(z), \quad n = 0, 1, 2, \ldots
\]  

(2.23)

with

\[
p_{n,t}(z) = \sum_{i=2}^{2n+1} \frac{(2\pi)^{i-1}}{i!} B_i \left( \frac{t}{2\pi} \right) z^{i-1}
\]  

(2.24)

and

\[
s_{n,t}(z) = \frac{(-1)^n}{\pi} \sum_{k=1}^{\infty} \frac{z^{2n} (z \cos(kt) + \frac{1}{k} z^2 \sin(kt))}{k^{2(n+1)} (z^2 + k^2)}.
\]  

(2.25)

**Proof** For \( n = 0 \) the relation (2.23) follows directly from (2.15). Assume that for some \( n \geq 0 \) the relation (2.23) holds. Using (2.13) we have

\[
s_{n,t}(z) = \frac{(-1)^n}{\pi} \sum_{k=1}^{\infty} \frac{z^{2(n+1)} (z \cos(kt) + \frac{1}{k} z^2 \sin(kt))}{k^{2(n+1)} (z^2 + k^2)} + \frac{(-1)^n}{\pi} \sum_{k=1}^{\infty} \frac{z^{2n} (z \cos(kt) + \frac{1}{k} z^2 \sin(kt))}{k^{2(n+1)}},
\]

i.e.,

\[
s_{n,t}(z) = s_{n+1,t}(z) + b_{n,t}(z),
\]  

(2.26)
where
\[ b_{n,t}(z) = \frac{(-1)^n}{\pi} z^{2n+1} \sum_{k=1}^{\infty} \frac{\cos(kt)}{k^{2(n+1)}} + \frac{(-1)^n}{\pi} z^{2n+2} \sum_{k=1}^{\infty} \frac{\sin(kt)}{k^{2n+3}}. \]

Using the formulas from [1], formula 23.1.18 we know that
\[ \sum_{k=1}^{\infty} \frac{\cos(kt)}{k^{2(n+1)}} = \frac{2(2\pi)^{2(n+1)} B_{2(n+1)}(t/(2\pi))}{(-1)^n 2(2n + 1)!} \]
and
\[ \sum_{k=1}^{\infty} \frac{\sin(kt)}{k^{2n+3}} = \frac{2(2\pi)^{2n+3} B_{2n+3}(t/(2\pi))}{(-1)^{n+2} 2(2n + 3)!}. \]

Hence it follows that
\[ b_{n,t}(z) = \frac{z^{2n+1}(2\pi)^{2n+1} B_{2n+2}(t/(2\pi))}{(2n + 2)!} + \frac{z^{2n+2}(2\pi)^{2n+2} B_{2n+3}(t/(2\pi))}{(2n + 3)!}. \]

Inserting this in (2.26) and using (2.23) we complete the proof of the statement.

2.1 The application to the \( \psi_1 \)-function

Observe that \( q_0(z) = \psi_1(2\pi z)/(2\pi) \) and \( \psi_1(z) \) admits a Maclaurin series expansion which can virtually be used to evaluate \( q_0(A) \). The following classical result provides the Maclaurin expansion of \( \psi_1(z) \).

**Theorem 1** ([1], formula 23.1.1) *It holds*
\[ \psi_1(z) = \phi_1(z)^{-1} = \sum_{k=0}^{+\infty} \frac{B_k}{k!} z^k, \quad |z| < 2\pi, \]
*where \( B_k \) denotes the \( k \)th Bernoulli number.*

Different rational approximations of \( \psi_1(z) \) can be derived from the Fourier series expansion of \( r_t(z) \). It turns out that such a series representation is also related with the Mittag-Leffler expansion of \( q_0(z) \).

Specifying the formulas and representations obtained above to the function \( \psi_1(A) \) we obtain the following. Using the formula (2.17) we have
\[ q_t(A) = \frac{1}{2\pi} I + \frac{t - \pi}{2\pi} A + A y_t(A) \]
and using (2.21) we find that
\[ q_t(A) = \frac{1}{2\pi} I_d + \frac{t - \pi}{2\pi} A + \frac{1}{\pi} \sum_{k=1}^{\infty} A^2 \cos(kt)(A^2 + k^2 I_d)^{-1} + \]
\[ + \frac{1}{\pi} \sum_{k=1}^{\infty} \frac{1}{k} A^3 \sin(kt)(A^2 + k^2 I_d)^{-1}, \quad 0 \leq t \leq \tau = 2\pi, \]
which implies

$$\psi_1(A) = 2\pi q_0(A/(2\pi)) = I_d - \frac{1}{2}A + 2\sum_{k=1}^{\infty} \left( \frac{A}{2\pi} \right)^2 \left( \frac{A}{2\pi} \right)^2 + k^2 I_d)^{-1}.$$  \hspace{1cm} (2.29)

Relation (2.29) is the first member of our family of rational approximations of $\psi_1(A)$.

This result may be improved by applying repeatedly the same approach as above. Indeed using (2.27) and (2.23), (2.24), (2.25)

$$q_t(A) = \frac{1}{2\pi} I + \frac{t-\pi}{2\pi} A + \sum_{i=2}^{2n+1} \frac{(2\pi)^i}{i!} B_i \left( \frac{t}{2\pi} \right)^i A^i + \frac{(-1)^n}{\pi} \sum_{k=1}^{\infty} \frac{A^{2n+1}}{k^{2n}} (A \cos(kt) + \frac{1}{k} A^2 \sin(kt)) (A^2 + k^2 I)^{-1}.$$  \hspace{1cm} (2.30)

Setting $t = 0$ we get

$$q_0(A) = \frac{1}{2\pi} I - \frac{1}{2} A + \sum_{i=2}^{2n+1} \frac{(2\pi)^i}{i!} B_i A^i + \frac{(-1)^n}{\pi} \sum_{k=1}^{\infty} \frac{A^{2n+2}}{k^{2n}} (A^2 + k^2 I)^{-1}.$$  \hspace{1cm} (2.30)

Since for $n > 1$ the odd Bernoulli numbers $B_n$ are zeroes we have

$$\sum_{i=2}^{2n+1} \frac{(2\pi)^i}{i!} B_i A^i = \sum_{i=0}^{n-1} \frac{(2\pi)^{2i+1}}{(2(i+1))!} B_{2(i+1)} A^{2(i+1)}.$$  \hspace{1cm} (2.30)

Hence, using $\psi_1(A) = \phi_1(A)^{-1} = 2\pi q_0(A/(2\pi))$ we arrive at the main result of the present paper

**Theorem 2** For any fixed $n > 0$ it holds

$$\psi_1(A) = p_n(A) + 2(-1)^n \sum_{k=1}^{\infty} \left( \frac{A}{2\pi} \right)^{2(n+1)} \frac{1}{k^{2n}} \left( \frac{A}{2\pi} \right)^2 + k^2 I_d)^{-1},$$  \hspace{1cm} (2.30)

where

$$p_n(A) = I_d - \frac{1}{2} A + \sum_{i=0}^{n-1} A^{2(i+1)} \frac{B_{2(i+1)}}{(2(i+1))!}.$$  \hspace{1cm} (2.30)

Observe that $p_n(A)$ is the classical approximation of $\psi_1(A)$ given in Theorem 1. Also notice that the rate of convergence of the series is the same as for the series $\sum_{k=1}^{\infty} k^{-2(n+1)}$ where $2n$ is the degree of the polynomial approximation. The above result presents a rational correction of this approximation aimed to improve its convergence properties. Specifically, based on Theorem 2 we introduce the following family $\{\psi_{n,s}(A)\}_{(n,s) \in \mathbb{N} \times \mathbb{N}}$ of mixed polynomial-rational approximations of $\psi_1(A)$:

$$\psi_{n,s}(A) = p_n(A) + 2(-1)^n \left( \sum_{k=1}^{s} \frac{1}{k^{2n}} \left( \frac{A}{2\pi} \right)^2 + k^2 I_d \right) \left( \frac{A}{2\pi} \right)^{2(n+1)}.$$  \hspace{1cm} (2.30)
Remark 1 The above approach based on the Fourier series expansion of $q_1(z)/z$ encompasses some rational approximations of $\psi_1(z)$ which can also be derived by applying Mittag-Leffler pole decomposition (see, e.g., [4] for a concise, hands-on presentation) to the function $q_0(z)$. More precisely, let us apply formula (7.54) in [4] to $q_0(z) = \psi(2\pi z) = \frac{2\pi z}{e^{2\pi z} - 1}$ with $p = 1$. The poles of our function are $\{ik\}_{k \in \mathbb{Z} \setminus \{0\}}$ and the corresponding residues are readily seen to be $\{ik\}_{k \in \mathbb{Z} \setminus \{0\}}$ as well. So we have

$$q_0(z) = q_0(0) + zq'(0) + \sum_{k \in \mathbb{Z} \setminus \{0\}} \frac{ikz^2/(ik)^2}{z - ik}$$

$$= 1 - \pi z + \sum_{k \in \mathbb{Z} \setminus \{0\}} -\frac{iz^2}{k(z - ik)}$$

$$= 1 - \pi z + \sum_{k=1}^{\infty} \frac{2z^2}{z^2 + k^2},$$

which is exactly formula (2.14) with $t = 0$. At this point we can apply (2.13) and proceed as above (again with $t = 0$) to obtain:

$$q_0(z) = 1 - \pi z + 2\sum_{k=1}^{\infty} z^2 \left( \sum_{i=0}^{n-1} (-1)^i \frac{z^{2i}}{k^{i+2}} + (-1)^n \frac{z^{2n}}{k^{2n}(z^2 + k^2)} \right)$$

$$= 1 - \pi z + 2\sum_{i=0}^{n-1} (-1)^i z^{2i+2} \sum_{k=1}^{\infty} \frac{1}{k^{i+2}} + 2(-1)^n z^{2n} \sum_{k=1}^{\infty} \frac{1}{k^{2n}(z^2 + k^2)}$$

$$= 1 - \pi z + 2\sum_{i=0}^{n-1} (-1)^i z^{2i+2} \zeta(2i + 2) + 2(-1)^n z^{2n} \sum_{k=1}^{\infty} \frac{1}{k^{2n}(z^2 + k^2)}, \quad (2.31)$$

where $\zeta$ denotes the Riemann zeta function. Now recall that even-indexed Bernoulli numbers are characterized by the relation

$$B_{2\ell} = \frac{(-1)^{\ell-1}(2\ell)!}{2^{2\ell-1}\pi^{2\ell}} \zeta(2\ell) \quad (2.32)$$

(see, e.g., [17], item 9.616), whereas the odd-indexed ones are zero except for $B_1 = -\frac{1}{2}$. From (2.32) we deduce

$$\zeta(2\ell) = \frac{B_{2\ell}(-1)^{\ell-1}2^{2\ell-1}\pi^{2\ell}}{(2\ell)!} \quad (2.33)$$

and by plugging (2.33) with $\ell = i + 1$ in equation (2.31) we obtain

$$q_0(z) = 1 - \pi z + \sum_{i=0}^{n-1} \frac{B_{2i+2}(2\pi z)^{2i+2}}{(2i + 2)!} + 2(-1)^n z^{2n} \sum_{k=1}^{\infty} \frac{1}{k^{2n}(z^2 + k^2)},$$

which is essentially the same mixed polynomial-rational development as in Theorem 2, in scalar form.
2.2 Numerical experiments

We begin by testing the behavior of mixed approximations applied to scalar (real or complex) arguments.

In Figs. 1 and 2 we show the plot over the interval $[-3\pi, 3\pi]$ of the functions $g(x) = \psi_1(x) = \frac{x}{e^x - 1}$, its polynomial approximation $f(x) = \psi_{20,0}(x)$ and its rational approximation $r(x) = \psi_{4,16}(x)$. Clearly, the rational approximation performs better when the points are close to the border of the convergence disk of the Maclaurin series given in Theorem 1. This same phenomenon can be observed in the complex plane. In Fig. 3 we illustrate the absolute error of rational approximation at complex points $x = a + ib$ with $a, b \in [-3\pi, 3\pi]$.
Remark 2  It is interesting to compare the complexity of computing a mixed approximation $\psi_{n,s}(A)$ and a classical rational approximation to $\phi_1(A)$, such as diagonal $(k, k)$—Padé, when $A$ is a large structured matrix.

Suppose for instance that $A$ has size $d \times d$ with quasiseparable rank $h$, in which case structured inversion of $A$ requires $O(h^2d)$ operations. Recall that a polynomial of degree $k$ applied to $A$ yields a structured matrix of quasiseparable rank $hk$. Then the cost of applying a $(k, k)$—Padé approximation $N(z)/D(z)$ to $A$ is dominated by the computation of $N(A)D(A)^{-1}$, which requires $O(h^2k^2d)$ operations. On the other hand, the evaluation of $\psi_{n,s}(A)$, where $n$ is supposed to be small and constant, is dominated by the computation of the $s$ rational terms, whose cost amounts to $O(sh^2d)$ operations. In other words, the computational cost tends to grow quadratically with the degree of a Padé approximation, whereas it grows linearly with the degree of a mixed approximation.

Remark 3  A widespread approach to the computation of exponential and $\phi_\ell$ functions combines polynomial or Padé approximation with a few steps of scaling-and-squaring [19]. In principle, scaling-and-squaring may also be applied to our mixed polynomial-rational approximation, scaling the function argument by a suitable power of 2 and then making use of the squaring formulas

$$\psi_1(2z) = \frac{2\psi_1(z)}{e^z + 1} = \frac{2\psi_1(z)^2}{z + 2\psi_1(z)}.$$  \hspace{1cm} (2.34)

See Fig. 4 for a numerical example.
Fig. 4 Absolute error for the approximation of the function \( \psi_1(z) \) in the complex plane, represented in \( \log_{10} \) scale. Here Padé approximations are obtained as the reciprocals of the \((6, 6)\)-Padé approximations to \( \phi_1(z) \) given by \texttt{padeapprox} in Chebfun [11] (without scaling) and by \texttt{phipade} in EXPINT [6] (with scaling). Mixed approximations are computed as \( \psi_{3,20}(z) \). The last two figures show results obtained using Carathéodory-Fejér approximation implemented as in [28] (left) and as in Chebfun (right), both without scaling.

Since mixed approximation is accurate on a larger domain than polynomial or Padé, it requires a smaller number of squaring steps. This is a useful property, because in some cases each squaring step may contribute to significant error accumulation (see, e.g., [3, 10] and references therein).

Unfortunately, the application of (2.34) when computing \( \psi_1(A) \) or \( \psi_1(A)v \) requires the inversion of the matrix \( A + 2\psi_1(A) \) or of \( e^A + I \). Note however that the matrix \( e^A + I \) will generally be well conditioned for symmetric \( A \), even when \( A \) has negative eigenvalues.

In the next tables we compare the accuracy of polynomial and rational approximations for computing both the matrix function \( \psi_1(A) \) and the vector \( \psi_1(A)v \), where
$A \in \mathbb{R}^{d \times d}$ is symmetric and $b \in \mathbb{R}^d$. As claimed in the introduction we are interested in the case where $A$ is structured so that we can assume that a linear system $Ax = f$ can be solved in linear time (possibly up to logarithmic factors) with a linear storage. All of our numerical tests are performed using MATLAB R2019a for comparison purposes we use the Padé approximation to the $\phi_1$-function as implemented in the EXPINT package [6].

Our test suite is as follows:

1. $A$ is the $900 \times 900$ block tridiagonal matrix obtained by discretizing the 2-dimensional Laplace operator with the usual 5-point rule on an $30 \times 30$ grid, that is, $A = \text{gallery('poisson',30)}$;
2. $A$ is the $d \times d$ Toeplitz tridiagonal matrix generated by the command $A = \text{gallery('tridiag',d,-1,4,-1)}$, i.e.,

$$A = \begin{bmatrix}
4 & -1 & 0 & \ldots & 0 \\
-1 & 4 & -1 & \ddots & \vdots \\
0 & \ddots & \ddots & \ddots & 0 \\
\vdots & \ddots & \ddots & \ddots & -1 \\
0 & \ldots & 0 & -1 & 4
\end{bmatrix}.$$

3. $A$ is the order one $d \times d$ quasiseparable matrix generated as $A = 0.7 * \text{inv(gallery('tridiag',d,d/2,[d:-1:1],d/2))}$; that is:

$$A = \begin{bmatrix}
d & d/2 & 0 & \ldots & 0 \\
d/2 & d - 1 & d/2 & \ddots & \vdots \\
0 & \ddots & \ddots & \ddots & 0 \\
\vdots & \ddots & d/2 & 2 & d/2 \\
0 & \ldots & 0 & d/2 & 1
\end{bmatrix},$$

with even $d$.
4. $A$ is the $d \times d$ Kac-Murdock-Szegö Toeplitz matrix such that $A_{ij} = 0.8^{|i-j|}$. It can be generated in MATLAB as $A = \text{gallery('kms',d,0.8)}$;
5. $A$ is the $100 \times 100$ “smoke matrix” generated as $A = \text{gallery('smoke',100)}$. This is a nonsymmetric matrix.

For comparison purposes, when $A$ is symmetric an accurate approximation of $\psi(A)$ is determined by computing the spectral decomposition of $A$. If $A$ is nonsymmetric, an accurate approximation of $\psi(A)$ is determined either via eigendecomposition or through the $\text{expm}$ function, using the Advanpix multiprecision package for MATLAB [2], set to work with 64 digits.

---

1 The MATLAB code used for the numerical tests is available at http://people.cs.dm.unipi.it/boito/psi1.zip.
Table 1 Errors for Example (1) and bounds from (4.46). Polynomial approximation fails in this example (i.e., it yields errors $\gg 1$)

| $k$ | $\text{err}._{(k,k)}$-Padé | $s$ | $\text{err}._{\psi_{3,s}}$ | $\|\varepsilon_{3,s}\|_2/\|\psi_1(A)\|_2$ |
|-----|----------------|-----|----------------|----------------------------------|
| 5   | 4.08e$-7$   | 10  | 1.34e$-7$   | 1.36e$-7$                        |
| 6   | 9.59e$-9$   | 20  | 1.27e$-9$   | 1.28e$-9$                        |
| 7   | 1.69e$-10$  | 30  | 7.92e$-11$  | 7.94e$-11$                       |
| 10  | 7.00e$-14$  | 40  | 1.09e$-11$  | 1.09e$-11$                       |
| 20  | 6.07e$-14$  | 50  | 2.32e$-12$  | 2.33e$-12$                       |
| 30  | 5.85e$-14$  | 100 | 7.92e$-15$  | 1.82e$-14$                       |

For any given $n \geq 1$ the polynomial and rational approximations of $\phi_1(A)^{-1}$ are $\psi_{n,0}(A)$ and $\psi_{m,n-m}(A)$, respectively. The corresponding normwise relative errors are

$$\text{err}._p = \frac{\|\psi(A) - p_n(A)\|}{\|\psi(A)\|}, \quad \text{err}._{\psi_{n,s}} = \frac{\|\psi(A) - \psi_{n,s}(A)\|}{\|\psi(A)\|}.$$

Tables 1, 2, 3, 4, and 5 show the errors evaluated for polynomial, rational Padé and mixed approximations (polynomial and mixed are applied without scaling, Padé involves scaling) applied to the test matrices. Padé approximations are computed by inverting the approximation of $\phi_1(A)$ given by EXPINT; in these examples $\phi_1(A)$ is generally well conditioned.

At this time we are just interested in comparing the accuracy of different approximations without incorporating fast linear solvers in our code. However, we point out that for the considered examples fast solvers exist that are expected to behave like Gaussian-elimination-based algorithms. Observe that in Example (3) for $d = 2056$ the eigenvalues are out of the disk centered at the origin of radius $2\pi$ and this explains the divergent behavior of the polynomial approximation.

In order to investigate further the behavior of the different approximations under the occurrence of possibly complex eigenvalues we have compared the accuracy of polynomial and rational methods for approximating the matrix $\psi_1(A)$ where $A = \gamma F$ and $F$ is the generator of the circulant matrix algebra, that is, the companion matrix associated with the polynomial $z^d - 1$. Since we know that the eigenvalues of $F$ lie

Table 2 Errors for Example (2)

| $d$ | $\text{err}._{p_{53}}$ | $\text{err}._{(7,7)}$-Padé | $\text{err}._{\psi_{3,50}}$ |
|-----|----------------|----------------|----------------|
| 256 | 2.29e$-1$ | 2.92e$-11$ | 7.54e$-13$ |
| 512 | 2.29e$-1$ | 2.92e$-11$ | 7.54e$-13$ |
| 1024| 2.30e$-1$ | 2.92e$-11$ | 7.54e$-13$ |
| 2048| 2.30e$-1$ | 2.92e$-11$ | 7.54e$-13$ |
on the unit circle the parameter \( \gamma \) is used to estimate the convergence of the methods when the magnitude of eigenvalues increase. Table 6 illustrates the errors for the case \( d = 1024 \). The divergence of the polynomial approximation for \( \gamma \geq 8 \) is in accordance with the theoretical results.

For \( \gamma = 64 \) we consider in Table 7 the errors generated by rational approximations of increasing order. The table suggests that rational approximations of higher orders are suited to give accurate results independently of the magnitude of the eigenvalues of \( A \).

We conclude this section with an experiment on accuracy and timings for adjacency matrices. The matrix \( A \in \mathbb{R}^{d \times d} \) is chosen as the adjacency matrix of a small-world graph, generated using the CONTEST toolbox for MATLAB [29] via the command \( A = \text{smallw}(d, 2, 0.2) \) and normalized so as to have \( \| A \|_2 = 6 \). This is a sparse symmetric matrix formed by a pentadiagonal term plus additional entries in random positions. Table 8 shows accuracy and timings for the approximation of \( \psi_1(A)v \), where \( v \in \mathbb{R}^d \) is the vector with all entries equal to one. The solution of the \( s \) linear systems required in the mixed approximation is carried out via MATLAB’s backslash sparse solver. Polynomial approximation fails in this case, i.e., yields a relative error larger than 1. Here we also include in the comparison the approximation of \( \psi_1(A) \) through the built-in MATLAB function \( \expm \). Figure 5 shows the behavior of computation times in logarithmic scale: data from mixed approximation clearly yield a smaller slope than Padé or \( \expm \).

### Table 3 Errors for Example (3)

| \( d \)  | \( err_{p53} \)     | \( err_{(7, 7)} \)-Padé | \( err_{\psi_{3,50}} \) | \( err_{\psi_{3,50}} \) with scaling |
|---------|---------------------|--------------------------|-------------------------|-------------------------------------|
| 256     | 1.60e-12            | 1.60e-12                 | 1.60e-12                | 1.60e-12                            |
| 512     | 5.55e-12            | 2.55e-12                 | 2.55e-12                | 2.55e-12                            |
| 1024    | 2.14e-4             | 1.97e-11                 | 1.97e-11                | 1.97e-11                            |
| 2048    | 4.33e+173           | 6.46e-11                 | 1.36e-2                 | 7.89e-10                            |

### Table 4 Errors for Example (4)

| \( d \)  | \( err_{p53} \)     | \( err_{(7, 7)} \)-Padé | \( err_{\psi_{3,50}} \) |
|---------|---------------------|--------------------------|-------------------------|
| 256     | 5.37e-15            | 3.06e-13                 | 2.38e-14                |
| 512     | 6.21e-15            | 3.14e-13                 | 2.43e-14                |
| 1024    | 7.32e-15            | 3.16e-13                 | 2.45e-14                |
| 2048    | 1.15e-14            | 3.17e-13                 | 2.46e-14                |
3 An application to a multi-degree of freedom system

As an example of application of the $\psi_1$ function to a concrete physical problem, we consider a multi-degree of freedom system suggested in [15], Section 9.2. It is a mass-spring oscillating system of $N$ masses $m_1, \ldots, m_N$ as in the following diagram:

![Diagram of a multi-degree of freedom system](image)

The elastic constants of the $N + 1$ springs are denoted as $k_1, \ldots, k_{N+1}$, whereas $\lambda_1, \ldots, \lambda_N$ are the friction coefficients associated with each mass.

The system is modeled by the second-order ordinary differential equation

$$M \frac{d^2}{dt^2} x(t) + C \frac{d}{dt} x(t) + K x(t) = f, \quad t \in [0, \tau],$$

where $M, C, K$ are the mass, damping and stiffness matrices, respectively. The vector $f$ is the external force, assumed to be constant, and $x(t)$ is the displacement vector, that is, $x_i(t)$ gives the position of the $i$-th mass with respect to a local reference system. Both $f$ and $x(t)$ are unknown. Such a setup could be useful, for instance, if we need to determine electric charges associated with $m_1, \ldots, m_N$: these can be obtained by applying a uniform electric field to the system and finding the constant force exerted on the masses. To this end, we can choose the initial position and velocity of the masses, that is, $x(0)$ and $\frac{d}{dt} x(0)$, and let the system evolve for a time $\tau$. Then the final position and velocity $x(\tau)$ and $\frac{d}{dt} x(\tau)$ are measured. Equipped with these data, we seek to determine $f$.

### Table 5

| err$_P$$_{p53}$ | err$_\psi$(7, 7)-Padé | err$_\psi$$_{3,50}$ |
|-----------------|---------------------|---------------------|
| 2.28e−16        | 1.14e−13            | 1.36e−16            |

### Table 6

| $\gamma$ | err$_P$$_{p53}$ | err$_\psi$$_{3,50}$ | err$_\psi$$_{3,50}$ with scaling |
|----------|-----------------|---------------------|----------------------------------|
| 2        | 1.88e−19        | 1.56e−17            | 1.56e−17                         |
| 4        | 6.92e−18        | 2.25e−15            | 2.25e−12                         |
| 8        | 8.44e+10        | 2.90e−13            | 2.90e−13                         |
| 16       | 1.58e+42        | 4.46e−11            | 3.45e−13                         |
| 32       | 3.11e+73        | 2.68e−9             | 4.49e−12                         |
| 64       | 2.046e+105      | 5.86e−7             | 4.09e−12                         |

Here $\phi_1(A)$ may be very ill-conditioned for large $\gamma$, so the Padé approximation is not reported.
Table 7  Errors for rational approximations of increasing orders

| γ | $err_{\gamma 3,50}$ | $err_{\gamma 3,100}$ | $err_{\gamma 3,200}$ | $err_{\gamma 3,400}$ |
|---|---|---|---|---|
| 64 | 5.86e−7 | 4.65e−9 | 5.87e−11 | 2.24e−11 |

In this experiment, the physical system is simulated numerically, with an arbitrary choice of $f$, to determine an “exact” solution $x(t)$ and thus the initial and final values of position and velocity of the masses. This procedure guarantees that these boundary conditions, although overdetermined, are compatible. The goal is to retrieve the value of the external force $f$.

Now, equation (3.35) can be rewritten as a first-order problem as follows:

$$
\frac{d}{dt}y(t) = Ay(t) + p,
$$

where

$$
y(t) = \begin{bmatrix} x(t) \\ \frac{d}{dt}x(t) \end{bmatrix}, \quad A = \begin{bmatrix} 0 & I \\ -M^{-1}K & -M^{-1}C \end{bmatrix}, \quad p = \begin{bmatrix} 0 \\ f \end{bmatrix},
$$

as the mass matrix $M$ can be safely assumed to be invertible. Consider boundary conditions

$$
y(0) = \begin{bmatrix} x(0) \\ \frac{d}{dt}x(0) \end{bmatrix}, \quad y(\tau) = \begin{bmatrix} x(\tau) \\ \frac{d}{dt}x(\tau) \end{bmatrix},
$$

which are known from the simulation.

We now have a first-order differential problem defined by equation (3.36) with boundary conditions (3.37), and we seek to determine the vector $p$. Note that the computed $p$ is expected to be formed by a zero block followed by the sought value of $f$.

This problem happens to be of the same kind as the model problem (1.1), (1.2). As mentioned in the introduction, the vector $p$ can be computed explicitly via (1.7). The main computational effort when applying (1.7) consists in computing the product of $\psi_1(\tau A)$ times a vector. Here this is done using our mixed polynomial-rational approximation (2.30) for $\psi_1(\tau A)$, which requires to solve several linear systems with

Table 8  Errors and timings (in seconds) for approximation of $\psi_1(A)v$, where $A$ is a $d \times d$ small-world adjacency matrix and $v = [1, 1, \ldots, 1]^T$

| $d$ | $err_{p3}$ time | $err_{(6, 6)}$-Padé time | $err_{\psi 3,50}$ time | $err_{\expm}$ time |
|---|---|---|---|---|
| 1000 | 4.23e−2 | 9.32e−4 | 6.66e−13 | 4.20 | 1.46e−12 | 3.72e−1 | 9.20e−13 | 1.21e−1 |
| 2000 | 3.81e−2 | 1.52e−3 | 6.11e−13 | 30.53 | 1.30e−12 | 2.01 | 2.19e−12 | 7.81e−1 |
| 3000 | 3.96e−2 | 4.81e−3 | 6.32e−13 | 110.48 | 1.38e−12 | 2.10 | 1.81e−12 | 2.42 |
| 4000 | 4.00e−2 | 5.01e−3 | 6.42e−13 | 265.91 | 1.37e−12 | 3.31 | 1.04e−12 | 5.66 |
| 5000 | 4.05e−2 | 7.30e−3 | 6.49e−13 | 517.07 | 1.40e−12 | 5.16 | 1.79e−12 | 12.06 |
| 6000 | 3.89e−2 | 8.84e−3 | 6.39e−13 | 874.43 | 1.38e−12 | 7.06 | 3.99e−12 | 18.85 |
| 7000 | 3.86e−2 | 1.04e−2 | 6.35e−13 | 1.36e+3 | 1.35e−12 | 9.98 | 4.67e−12 | 31.15 |
coefficient matrices given by diagonal shifts of a scalar multiple of $A^2$. Understanding the structure of $A$ and $A^2$ may help solve such linear systems via fast methods, rather than applying a slower, general-purpose solver.

With the hypotheses outlined above, the mass and the damping matrices are diagonal:

$$M = \text{diag}(m_1, m_2, \ldots, m_N), \quad C = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_N),$$

whereas the matrix $K$ has a symmetric tridiagonal form:

$$K = \begin{bmatrix}
  k_1 + k_2 & -k_2 & \cdots & \cdots & -k_3 \\
  -k_2 & k_2 + k_3 & -k_3 & \cdots & \cdots \\
  \cdots & \cdots & \ddots & \ddots & \cdots \\
  \cdots & \cdots & \ddots & \ddots & \cdots \\
  -k_{N-1} & k_{N-1} + k_N & -k_N & -k_N & k_N + k_{N+1}
\end{bmatrix}.$$ 

Clearly the matrix $A$ inherits a sparse/banded structure, which allows for a computationally cheap application of the mixed approximation formula. Indeed, the matrix $A^2$
has a $2 \times 2$ block structure with tridiagonal blocks, so we can employ the well-known formula

$$
\begin{bmatrix}
A & B \\
C & D
\end{bmatrix}^{-1} = \begin{bmatrix}
A^{-1} + A^{-1}BS^{-1}CA^{-1} & -A^{-1}BS^{-1} \\
-S^{-1}CA^{-1} & -S^{-1}
\end{bmatrix}
$$

(3.38)

and perform inversions using quasiseparable structure. In particular, note that the Schur complement $S = D - CA^{-1}B$ has quasiseparable rank at most three. Therefore, the computational cost of this approach is $O(N)$. While in general inversion methods based on the Schur complement may suffer from stability issues, such issues are not observed in this specific example.

**Remark 4** Of course the structure of the matrix $A$ can be parameterized in different ways. For instance, one may observe that $A$ is banded and therefore also quasiseparable; note, however, that the bandwidth and the quasiseparability order increase with $N$. On the other hand, the quasiseparable generators are sparse themselves, which in practice may lead to computational savings.

In addition, if the masses in the physical system are all equal and have the same friction coefficient, and the springs all have the same elastic constant, then $A$ exhibits a low-order Toeplitz-like structure, which allows for fast inversion of $A^2/2\pi + k^2I$.

In this numerical test we take $\tau = 1$ and $m_i = 1$, $k_i = 0.3$, $\lambda_i = 0.1$ for all indices $i$. As initial conditions for $t = 0$ we choose a displacement of 0.5 for all masses and zero velocity. The constant external force is set to 0.5, that is, $f = [0.5, \ldots, 0.5]^T$.

In order to simulate the evolution of the physical model, we need to integrate the differential equation (3.36): a preliminary computation via the MATLAB command `ode45`, with absolute and relative tolerances set at $1e^{-13}$, yields the boundary condition at $t = \tau$. With this setup we compute the vector $p$ via mixed approximation and compare it to the “exact” one. The methods examined in this example are:

- unstructured mixed polynomial-rational approximation (that is, computation of $\psi_{3,10}$ in (2.30) without taking advantage of the structure of $A$),
- structured block mixed polynomial-rational approximation (that is, computation of $\psi_{3,10}$ in (2.30), where matrix inversion is performed via (3.38) in combination with quasiseparable inversion algorithms),
- approximation of $\psi_1(A)$ via `EXPIINT`,
- approximation of $\psi_1(A)$ via `expm`.

The results are shown in Tables 9, 10, 11, and 12, for $N = 50, 100, 500, 1000$. The tables report the norm of the $(1 : N)$-block of the computed vector $p$, which should ideally be zero, and the absolute and relative errors on the $(N + 1 : 2N)$-block corresponding to the force vector. The quality of the `expm` approximation tends to

---

2 A detailed presentation of quasiseparable matrix structure is beyond the scope of this paper; we refer the interested reader to the book [13]. For the purpose of this example let us recall that quasiseparability is a kind of matrix rank structure that allows for inversion in $O(N)$ operations, and that banded matrices belong to the quasiseparable class.
deteriorate for growing $N$, whereas both the structured and the unstructured mixed approximation are as accurate as EXPINT.

4 Bounds on the decay of the reciprocal of the $\phi_1$-function

In this section we investigate the approximate rank structure of $\psi_1(A)$ for a suitable $A$. Specifically, as an application of Theorem 2 we can deduce a priori bounds on the decay of the $\psi_1$-function applied to symmetric banded matrices.

Now, let $A \in \mathbb{R}^{d \times d}$ be a symmetric banded matrix. Denote as $m$ the half-bandwidth of $A$, that is, $A_{i,j} = 0$ if $|i-j| > m$. It is well known that the off-diagonal entries of $\psi_1(A)$ exhibit a decay behavior in absolute value (the same is true of any other function of $A$ that is well defined and sufficiently regular [5]). We can use the $(n, s)$-mixed polynomial-rational approximation (2.30) to give bounds on this decay behavior.

Define

$$ r_{n,s}(z) = 2(-1)^n \left( \frac{z}{2\pi} \right)^{2(n+1)} \sum_{k=1}^{s} \frac{1}{k^{2n} \left( \left( \frac{z}{2\pi} \right)^2 + k^2 \right)} , $$

$$ p_n(z) = 1 - \frac{1}{2} z + \sum_{i=0}^{n-1} z^{2(i+1)} \frac{B_{2(i+1)}}{(2(i+1))!} $$

which we will call the rational and the polynomial part of (2.30), respectively, and let

$$ \varepsilon_{n,s}(z) = \psi_1(z) - p_n(z) - r_{n,s}(z) $$

be the $(n, s)$-approximation error. We have

$$ |[\psi_1(A)]_{i,j}| \leq |[p_n(A)]_{i,j}| + |[r_{n,s}(A)]_{i,j}| + |[\varepsilon_{n,s}(A)]_{i,j}|. $$

Table 9 Errors for $N = 50$

| Approximation          | $\|p(1:N)\|_2$ | abs. err. on $f$ | rel. err. on $f$ |
|------------------------|----------------|------------------|------------------|
| Unstructured mixed     | 1.52e$-14$    | 1.06e$-14$       | 2.98e$-15$       |
| 2 $\times$ 2 QS mixed | 1.51e$-14$    | 1.05e$-14$       | 2.98e$-15$       |
| EXPINT                 | 1.51e$-14$    | 1.06e$-14$       | 2.99e$-15$       |
| expm                   | 1.77e$-13$    | 7.45e$-13$       | 2.11e$-13$       |

Table 10 Errors for $N = 100$

| Approximation          | $\|p(1:N)\|_2$ | abs. err. on $f$ | rel. err. on $f$ |
|------------------------|----------------|------------------|------------------|
| Unstructured mixed     | 1.52e$-14$    | 1.06e$-14$       | 2.13e$-15$       |
| 2 $\times$ 2 QS mixed | 1.51e$-14$    | 1.05e$-14$       | 2.11e$-15$       |
| EXPINT                 | 1.52e$-14$    | 1.09e$-14$       | 2.17e$-15$       |
| expm                   | 9.69e$-13$    | 3.88e$-12$       | 7.76e$-13$       |
Observe that \( p_n(A) \) is a banded matrix with half-bandwidth \( 2nm \). So, if we choose \( i, j \) such that \(|i - j| > 2nm\), then \(|[p_n(A)]_{i,j}| = 0\) and we only need to focus on the rational and error terms.

For the rational term, let us start by giving a bound on

\[
\tilde{r}_{n,s}(A) := \sum_{k=1}^{s} \frac{1}{k^{2n}} \left( \left( \frac{A}{2\pi} \right)^2 + k^2 I_d \right)^{-1}.
\]

The matrix \( A_k = \left( \frac{A}{2\pi} \right)^2 + k^2 I_d \) is positive definite with semi-bandwidth \( 2m \), and several exponential decay bounds for the inverse of a positive definite matrix have been proposed in the literature. Prop. 2.2 from [9], for instance, gives

\[
|[A_k^{-1}]_{i,j}| \leq C_k \lambda_k^{|i-j|},
\]

where

\[
a_k = k^2, \quad b_k = \left( \frac{\rho(A)}{2\pi} \right)^2 + k^2, \quad r_k = \frac{b_k}{a_k}, \quad \lambda_k = \left( \frac{\sqrt{r_k} - 1}{\sqrt{r_k} + 1} \right)^{1/2m}, \quad C_k = \max \left\{ a_k^{-1}, \frac{(1 + \sqrt{r_k})^2}{2a_k r_k} \right\},
\]

where \( \rho(A) \) is the spectral radius of \( A \) and \( 0 < a_k < b_k \) are such that the spectrum of \( A_k \) is contained in \([a_k, b_k]\). Therefore, we have

\[
\left| \sum_{k=1}^{s} \frac{1}{k^{2n}} \left( \left( \frac{A}{2\pi} \right)^2 + k^2 I_d \right)^{-1} \right|_{i,j} \leq \sum_{k=1}^{s} \frac{1}{k^{2n}} C_k \lambda_k^{|i-j|}
\]

Table 11  Errors for \( N = 500 \)

|                      | \( \|p(1:N)\|_2 \) | abs. err. on \( f \) | rel. err. on \( f \) |
|----------------------|---------------------|----------------------|----------------------|
| Unstructured mixed   | 1.52e−14            | 1.15e−14             | 1.03e−15             |
| 2 × 2 QS mixed       | 1.51e−14            | 1.06e−14             | 9.48e−16             |
| EXPINT               | 1.54e−14            | 1.31e−14             | 1.18e−15             |
| expm                 | 5.05e−11            | 1.74e−10             | 1.56e−11             |

Table 12  Errors for \( N = 1000 \)

|                      | \( \|p(1:N)\|_2 \) | abs. err. on \( f \) | rel. err. on \( f \) |
|----------------------|---------------------|----------------------|----------------------|
| Unstructured mixed   | 1.52e−14            | 1.26e−14             | 7.96e−16             |
| 2 × 2 QS mixed       | 1.51e−14            | 1.07e−14             | 6.75e−16             |
| EXPINT               | 1.57e−14            | 1.47e−14             | 9.28e−16             |
| expm                 | 3.25e−10            | 9.96e−10             | 6.30e−11             |
for all indices $i,j$. Now recall that $\left( A_{2\pi} \right)^{2(n+1)}$ is a banded matrix of bandwidth $2m(n + 1)$. So we have:

$$\left| [r_{n,s}(A)]_{i,j} \right| = 2 \left| \sum_{v=1}^{d} [\hat{r}_{n,s}(A)]_{i,v} \left( \frac{A}{2\pi} \right)^{2(n+1)} \right|_{v,j}$$

$$= 2 \left| \sum_{v=j-2m(n+1)}^{j+2m(n+1)} [\hat{r}_{n,s}(A)]_{i,v} \left( \frac{A}{2\pi} \right)^{2(n+1)} \right|_{v,j}$$

$$\leq 2 \left| \sum_{v=j-2m(n+1)}^{j+2m(n+1)} \left\| \frac{A}{2\pi} \right\|_{2}^{2(n+1)} \left( \sum_{k=1}^{s} \frac{C_k}{k^{2n}} |i-v| \right) \right|_{v,j}$$

$$= 2 \left\| \frac{A}{2\pi} \right\|_{2}^{2(n+1)} \sum_{v=j-2m(n+1)}^{j+2m(n+1)} \sum_{k=1}^{s} \frac{C_k}{k^{2n}} |i-v|,$$

where in the sums over $v$ it is understood that $1 \leq v \leq d$.

Let us now bound the error term. Define

$$\varepsilon_{n,s}(A) = 2\tilde{\varepsilon}_{n,s}(A) \left( \frac{A}{2\pi} \right)^{2(n+1)} \text{ where } \tilde{\varepsilon}_{n,s}(A) = \sum_{k=s+1}^{\infty} \frac{1}{k^{2n}} \left( \left( \frac{A}{2\pi} \right)^{2} + k^{2}I_{d} \right)^{-1}.$$ 

Therefore, we find that

$$||[\varepsilon_{n,s}(A)]_{i,j}| \leq \|\varepsilon_{n,s}(A)\|_{2} \leq 2\|\tilde{\varepsilon}_{n,s}(A)\|_{2} \left\| \frac{A}{2\pi} \right\|_{2}^{2(n+1)}.$$ (4.43)

Let us bound $\|\tilde{\varepsilon}_{n,s}(A)\|_{2}$. Let $A = UDU^{H}$ be the eigendecomposition of $A$ and denote the spectrum of $A$ as $\sigma(A)$; recall that $\sigma(A)$ is real. We have

$$\|\tilde{\varepsilon}_{n,s}(A)\|_{2} \leq \|\tilde{\varepsilon}_{n,s}(D)\|_{2} = \max_{x \in \sigma(A)} |\tilde{\varepsilon}_{n,s}(x)|$$ (4.44)

and moreover

$$|\tilde{\varepsilon}_{n,s}(x)| = \sum_{k=s+1}^{\infty} \frac{1}{k^{2n}} \left( \left( \frac{x}{2\pi} \right)^{2} + k^{2} \right)^{-1} \leq \sum_{k=s+1}^{\infty} \frac{1}{k^{2n+2}} = \zeta(2n+2) - \sum_{k=1}^{s} \frac{1}{k^{2n+2}},$$ (4.45)

from which we deduce

$$||[\varepsilon_{n,s}(A)]_{i,j}| \leq 2 \left\| \frac{A}{2\pi} \right\|_{2}^{2(n+1)} \left( \zeta(2n+2) - \sum_{k=1}^{s} \frac{1}{k^{2n+2}} \right),$$

where $\zeta(s)$ is the Riemann zeta function.

Summing up the following estimates are obtained for the entries of $\psi_{1}(A)$.

**Theorem 3** Let $A \in \mathbb{R}^{d \times d}$ be a symmetric banded matrix with half-bandwidth $m$. For all $(n, s) \in \mathbb{N} \times \mathbb{N}$ it holds

$$||[\psi_{1}(A)]_{i,j}| \leq ||[r_{n,s}(A)]_{i,j}| + ||[\varepsilon_{n,s}(A)]_{i,j}|, \quad |i - j| > 2mn,$$
where
\[
\| [r_{n,s}(A)]_{i,j} \| \leq 2 \left\| \frac{A}{2\pi} \right\|_{2}^{2(n+1)} \sum_{v=j-2m(n+1)}^{j+2m(n+1)} \sum_{k=1}^{s} \frac{C_{k}}{k^{2n+\lambda_{k}}} |i-v|
\]
and
\[
| [\varepsilon_{n,s}(A)]_{i,j} | \leq 2 \left\| \frac{A}{2\pi} \right\|_{2}^{2(n+1)} \left( \xi(2n+2) - \sum_{k=1}^{s} \frac{1}{k^{2n+\lambda_{k}}} \right),
\]
and \( C_{k} \) and \( \lambda_{k} \) are given in \((4.41), (4.42)\).

To illustrate the significance of these bounds we present in Fig. 6 numerical comparisons with other existing bounds deduced from [5]. Recall that these latter estimates are based on a theoretical result on the best degree-\( k \) polynomial approximation of the function \( \psi_{1}(z) \) on \([-1, 1]\) that cannot be explicitly computed. The corresponding best polynomial approximation error satisfies
\[
E_{k}(\psi_{1}) \leq \frac{2M(\chi)}{\chi^{k}(\chi - 1)}
\]
and depends on a parameter \( \chi \) that defines a Bernstein ellipse in the complex plane, where the function is analytic. For the case considered in Fig. 6 a good choice is \( \chi = 12 \). If the spectrum of the matrix is not contained in \([-1, 1]\), one needs to scale the matrix, that is, apply the function \( \psi_{1,\xi}(z) = \frac{\xi z}{e^{\xi z} - 1} \) to \( A/\xi \), for a suitable choice

![Fig. 6](image-url)
of $\xi$. Then the poles of the function closest to zero are at $\pm \frac{2\pi i}{\xi}$; the minor semi axis $\beta$ of the ellipse should be chosen slightly smaller than $\frac{2\pi}{\xi}$ and $\chi = \beta + \sqrt{\beta^2 + 1}$.

We see that the proposed mixed polynomial-rational approximation and the best polynomial approximation exhibit a similar decaying profile.

**Remark 5** The discussion in this section can also be used to estimate the approximation error for $\psi_{n,s}(A)$, under the hypothesis that $A$ is symmetric (although not necessarily banded). Namely, from (4.39) we have

$$\epsilon_{n,s}(A) = \psi_1(A) - \psi_{n,s}(A),$$

which, combined with (4.43), (4.44), (4.45), yields the normwise bound

$$\| \psi_1(A) - \psi_{n,s}(A) \|_2 \leq 2 \left\| \frac{A}{2\pi} \right\|_2^{2(n+1)} \left( \chi(2n + 2) - \sum_{k=1}^{s} \frac{1}{k^{2n+2}} \right).$$

(4.46)

Also note that the dependence of this bound on $A$ only involves $\|A\|_2$.

Numerical tests for Example 1 in Table 1 show that the bound (4.46) is actually quite tight, so in principle one may use this bound to estimate the parameter $s$ before computing $\psi_{n,s}(A)$. For instance, for the matrices in Example 2, with a given relative tolerance of $10^{-12}$, one may apply (4.46) for several values of $s$, as shown in Fig. 7,

![Fig. 7](image-url)  
**Fig. 7** Behavior, in logarithmic scale, of the bound (4.46) for the $256 \times 256$ matrix from Example 2. The horizontal red line is added as a visual aid to determine graphically a value of $s$ sufficient to attain a relative error smaller than $10^{-12}$.
and conclude that taking \( s = 48 \) is enough to approximate \( \psi_1(A) \) within the desired tolerance. This is consistent with the results in Table 2.

5 Conclusion and future work

In this paper we have introduced a family of rational approximations of the reciprocal of the \( \phi_1 \)-function encountered in exponential integration methods. This family extends customary approximations based on the Taylor series by showing better convergence properties. Therefore, the novel formulas are particularly suited when applied for computing the reciprocal of the \( \phi_1 \) matrix function of a structured matrix admitting fast and numerically robust linear solvers. Mixed polynomial-rational approximations of a meromorphic function based on the Dunford-Cauchy integral formula that are suited for computation with rank-structured matrices have been recently proposed in [24]. Theoretical and computational comparisons between the two families of approximations of \( \psi_1(z) = \phi_1(z)^{-1} \) is an ongoing work. Also a more detailed comparison of the approaches based on the Mittag-Leffler theorem and the rational Carathéodory-Fejér approximation [28] for evaluating \( \psi_1(z) \) would be interesting.

Another natural continuation of our results in Section 2 is the complete numerical solution of the inverse and nonlocal problems for differential equations as (1.1), (1.2) and (1.8).

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Declarations

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