THE COMPUTATION OF FUNCTIONS OF MATRICES BY TRUNCATED FABER SERIES

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Abstract. In this paper we consider a method based on Faber polynomials for the approximation of functions of real nonsymmetric matrices. Particular attention is devoted to some functions that occur in practical problem, such as $\exp(z)$, $\exp(-\sqrt{z})$, $\cos(\sqrt{z})$. Finally we give some numerical results on a test matrix arising from the discretization of a second order partial differential operator.

1. Introduction. Given a real matrix A of order N and a N-dimensional vector v, we consider the problem of the computation of

$$y = f(A)v, \tag{1.1}$$

where f is a given function that we suppose to be analytic in a certain domain of the complex plane containing the spectrum of A, $\sigma(A)$. That is, as well known,

$$f(A)v = \frac{1}{2\pi i}\int_\Gamma f(z)(zI - A)^{-1}v \; dz, \tag{1.2}$$

where Γ is the boundary curve of a piecewise smooth bounded region containing $\sigma(A)$ and where f is analytic.

This problem occurs in several applications, for instance in the solution of algebraic linear systems (where $f(z) = 1/z$) or of systems of differential equations, where the solution can be expressed in terms of (1.1). In the recent years, many studies have been devoted to polynomial approximations of (1.1). Consider, for instance, the methods proposed in [6], [7], [8], [9], [14], [17], [19], where approximations of (1.1) are obtained by projection into Krylov subspaces, defined with respect to A and v. Clearly, these procedures depend on v, and in some applications this may represent a disadvantage (see e.g. [14]).

Following a different line, in this paper we introduce a polynomial approach based on the approximation of f through Faber polynomials defined on a certain compact subset of the complex plane containing $\sigma(A)$. More precisely, given a certain compact $\Omega \subset \mathbf{C}$ such that $\sigma(A) \subseteq \Omega$, we consider a polynomial approximation

$$p_{m-1}(A)\, v \approx f(A)v,$$

where the polynomials p_{m-1}, $m \geq 1$, of degree $m-1$, are the truncating Faber series with respect to Ω and the function f (cf. e.g. [31]). So doing we extend procedures already considered in the contest of the solution of algebraic linear systems (see e.g. [10], [12], [33]). In the particular case that A is symmetric (skew-symmetric), $\sigma(A)$ is contained in a real (imaginary) interval, the associated Faber polynomials can be represented by scaled and translated Chebychev polynomials, and so the methods here considered also generalize some ideas already developed in [22], [23],[34], [35]. Another approach still based on complex polynomial approximation can be found in [26].

The main features of the approach here proposed, that make it competitive with other methods presented in the literature, are the following:

a) if $\sigma(A) \subseteq \Omega$ and f is analytic in Ω, the method converges (superlinearly if f is analytic everywhere). Moreover, depending on the position of the singularity of f outside Ω, the method can converge even if $\sigma(A) \nsubseteq \Omega$.

b) The use of Faber polynomials ensures the existence of a recurrence relation with a finite number of terms for the approximations $y_m = p_{m-1}(A)\,v$.

c) The definition of the iteration parameters for the above mentioned recursion is independent of v.

d) No explicit computation of any matrix functions must be performed (this is not the case of Krylov-projection methods).

e) The cost at each step is constant and substantially equal to that of an application of A.

The paper is organized as follows. In Sect. 2, we give an outline about the fundamental properties of polynomial methods for the computation of (1.1). Faber polynomials and series are described in Sect. 3, with particular attention to their asymptotic properties. In Sect.4 general error bounds for Faber series approximations is given. In Sect. 5 we consider some error bounds for some functions of practical interest. The implementation of the procedures is discussed in Sect. 6. Finally Sect. 7 contains some numerical tests involving a matrix arising from the discretization of a second order partial differential operator.

2. Background on polynomial methods. A polynomial method for the computation of (1.1) is a method yielding approximations of the type

$$y_m := p_{m-1}(A)\,v \approx f(A)v, \tag{2.1}$$

where $p_{m-1}(z)$ is a polynomial of degree at most $m-1$.

Given a compact subset $\Omega \subset \mathbf{C}$ such that $\sigma(A) \subseteq \Omega$, we are mainly interested in searching a sequence of polynomials $\{p_{m-1}(z)\}_{m\geq 1}$ such that the following holds:

$$\lim_{m\to\infty} \|f - p_{m-1}\|_{\Omega} = 0, \tag{2.2}$$

where $\|\ \|_{\Omega}$ denotes the supremum-norm on Ω . If A is diagonalizable i.e. XAX^{-1} is diagonal, we have immediately

$$\|\exp(A)v - p_{m-1}(A)\,v\|_2 \leq cond_2(X)\,\|f - p_{m-1}\|_{\Omega}\,\|v\|_2\,, \tag{2.3}$$

and so condition (2.2) ensures the convergence of the corresponding method (2.1). For the general case the following result (see e.g.[15]) holds:

Proposition 2.1. *Let $m(z) = \prod_{i=1}^{\nu}(z-\lambda_i)^{n_i}$ the minimal polynomial of A. The sequence $y_m = p_{m-1}(A)\,v$ converges to $f(A)v$ if and only if*

$$\lim_{m\to\infty} p_{m-1}^{(j)}(\lambda_i) = f^{(j)}(\lambda_i), \qquad 1 \leq i \leq \nu, \quad 0 \leq j \leq n_i - 1. \tag{2.4}$$

If A is diagonalizable then (2.4) reduces to

$$\lim_{m\to\infty} p_{m-1}(\lambda) = f(\lambda) \qquad for\ each\ \lambda \in \sigma(A)\,. \tag{2.5}$$

Moreover, if G is an open subset of $\mathbf{C}$ such that $\sigma(A) \subset G$, then the following condition is sufficient

$$\{p_{m-1}(\lambda)\}_{m\geq 1} \qquad \begin{array}{l} converges\ to\ f(\lambda),\ uniformly\ on \\ every\ compact\ subset\ contained\ in\ G. \end{array} \tag{2.6}$$

From these results we have that, if A is not diagonalizable, condition (2.2) does not ensure convergence. So in this case we must satisfy a condition stronger than (2.2). In this sense, we know (cf. [27]) that, if Ω ($\supseteq \sigma(A)$) contains infinitely many points and if $\left\{p^*_{m-1}(z)\right\}_{m\geq 1}$ is the sequence of polynomials of best uniform approximation of f on Ω, then the condition

$$\overline{\lim_{m\to\infty}} \|p_{m-1} - f\|_\Omega^{1/(m-1)} = \overline{\lim_{m\to\infty}} \left\|p^*_{m-1} - f\right\|_\Omega^{1/(m-1)}, \tag{2.7}$$

ensures the convergence of the method even if A is not diagonalizable (cf. also [12]). Indeed, if condition (2.7) holds, then (cf. e.g. [27]) there exists an open set G such that $\Omega \subset G$ (and therefore $\sigma(A) \subset G$) and such that $\{p_{m-1}(z)\}_{m\geq 1}$ converges uniformly on every compact subsets in G. In this situation the sequence $\{p_{m-1}(z)\}_{m\geq 1}$ is said *maximally convergent* to f on Ω, and the corresponding method *asymptotically optimal* with respect to Ω and f.

3. Faber polynomials and series. Let

$$\mathbf{M} := \left\{ \begin{array}{c} \Omega \subset \mathbf{C} : \Omega \text{ is compact, } \overline{\mathbf{C}} \setminus \Omega \text{ is simply connected and } \Omega \text{ contains} \\ \text{more than one point} \end{array} \right\}$$

Given $\Omega \in \mathbf{M}$, by the Riemann Mapping Theorem there exists a conformal surjection

$$\psi : \overline{\mathbf{C}} \setminus \{w : |w| \leq \gamma\} \to \overline{\mathbf{C}} \setminus \Omega, \qquad \psi(\infty) = \infty, \quad \psi'(\infty) = 1. \tag{3.1}$$

The constant γ is called the capacity of Ω. Let $\phi : \overline{\mathbf{C}} \setminus \Omega \to \overline{\mathbf{C}} \setminus \{w : |w| \leq \gamma\}$ be the inverse mapping of ψ. The j-th *(ordinary) Faber polynomial* is defined as the polynomial part of the Laurent expansion at ∞ of $[\phi(z)]^j$ (cf.[31],§2)

$$[\phi(z)]^j = z^j + \sum_{k=-\infty}^{j-1} \beta_{j,k} z^k, \qquad j \geq 0,$$

that is

$$F_j(z) := z^j + \sum_{k=0}^{j-1} \beta_{j,k} z^k, \qquad j \geq 0.$$

As well known, in the particular case that Ω coincides with the closure of the internal part of an ellipse or with an interval in the complex plane, Faber polynomials reduce to scaled and translated Chebychev polynomials [10].

Faber polynomials can be computed recursively (cf.[5]) from

$$\begin{gathered} F_0(z) = 1, \qquad F_1(z) = z - c_0, \quad \text{and, for } m \geq 2, \\ F_m(z) = (z - c_0) F_{m-1}(z) - (c_1 F_{m-2}(z) + ... + c_{m-1} F_0(z)) - (m-1) c_{m-1}. \end{gathered} \tag{3.2}$$

where the coefficients $c_0, c_1, ...$ are those of the Laurent expansion of the mapping ψ, that is

$$\psi(w) = w + c_0 + c_1 w^{-1} + c_2 w^{-2} .... \tag{3.3}$$

For any $R > \gamma$, let Γ_R be the equipotential curve

$$\Gamma_R := \{z : |\phi(z)| = R\}.$$

Moreover let us denote by Ω_R the bounded domain with boundary Γ_R. Let $\widehat{R} = \widehat{R}(f) > \gamma$ be the largest number such that a given function f is analytic on Ω_R for each $\gamma < R < \widehat{R}$ and has a (possible) singularity on $\Gamma_{\widehat{R}}$. The *(ordinary) Faber coefficients* with respect to the function f and the compact Ω are defined as

$$a_j(f) := \frac{1}{2\pi i}\int_{|w|=R} \frac{f(\psi(w))}{w^{j+1}}dw, \qquad j \geq 0, \quad \gamma < R < \widehat{R}. \tag{3.4}$$

From [31] (Theorem 1, p.167) we know that f can be expanded into a series of ordinary Faber polynomials in the following way

$$f(z) = \sum_{j=0}^{\infty} a_j(f) F_j\left(z\right), \tag{3.5}$$

and this representation is unique. Defining the polynomial sequence $\{p_{m-1}\left(z\right)\}_{m\geq 1}$ obtained by truncating the series (3.5), that is

$$p_{m-1}\left(z\right) := \sum_{j=0}^{m-1} a_j(f) F_j\left(z\right), \tag{3.6}$$

we can define the method

$$y_m := p_{m-1}\left(A\right) v. \tag{3.7}$$

From now on, we use the simplifyed notation $p_{m-1}\left(z\right) = \mathbf{F}_{m-1}(f)(z)$ to indicate (3.6). From [13], we know that the polynomial sequence (3.6) converges maximally on Ω to f (cf.(2.7)) and hence, if $\sigma(A) \subseteq \Omega$ the method (3.7) converges and is asymptotically optimal with respect to Ω and f. For the *asymptotic convergence factor* of the method, defined as

$$\overline{\lim_{m\to\infty}} \left[\|e_m\|^{1/m}\right], \qquad e_m := f(A)v - p_{m-1}\left(A\right) v, \tag{3.8}$$

it is known that

$$\overline{\lim_{m\to\infty}} \left[\|e_m\|^{1/m}\right] \leq \gamma / \widehat{R}(f), \tag{3.9}$$

even if A is not diagonalizable (see e.g. [10], [12], [26]). Relation (3.9) follows from the property of maximal convergence. By (3.9), for functions analytic in the whole complex plane, the rate of convergence of the method is superlinear, because of $\widehat{R}(f) = \infty$.

Besides the property of defining an asymptotically optimal method for the approximation of $f\left(A\right) v$, the use of Faber polynomials ensures the existence of a recurrence relation (cf.(3.2)) for computing the approximations $y_m = \mathbf{F}_{m-1}\left(f\right)(A)v$. Namely, the computation of the approximations y_m can be carried out recursively by

$$\begin{gathered} y_0 = 0, \qquad y_1 = a_0 v, \qquad y_2 = y_1 + \tfrac{a_1}{a_0}\left(A - c_0 I\right) r_0, \\ y_m = y_{m-1} + \tfrac{a_{m-1}}{a_{m-2}}\left(A - c_0 I\right) r_{m-2} - \tfrac{a_{m-1}}{a_{m-3}} c_1 r_{m-3} - .. - \tfrac{a_{m-1}}{a_0}\left(m-1\right) c_{m-2} r_0 \\ for \qquad m \geq 3, \end{gathered} \tag{3.10}$$

where $r_0 := y_1$, $r_k := y_{k+1} - y_k$ $(k \geq 1)$, and where the coefficients $a_k := a_k(f)$, $k \geq 0$, are defined by (3.4). Formula (3.10) follows by direct computation from (3.2) and (3.6). Of course, if the expansion (3.3) has a (a priori fixed) finite number of terms (and for example this is the case of the compact subsets bounded by ellipses) then the same will be true for relation (3.10).

REMARK 3.1. *If Ω is a compact such that $\sigma(A) \subseteq \Omega$ then*

$$\Omega_t := \left\{\lambda' : \lambda' = t\lambda, \lambda \in \Omega\right\}$$

contains $\sigma(tA)$, where t is a given scalar, and if

$$\psi(w) = w + \alpha_0 + \alpha_1 w^{-1} + ...$$

is the conformal mapping from $\overline{\mathbf{C}} \backslash \{w : |w| \leq \gamma\}$ into $\overline{\mathbf{C}} \backslash \Omega$ with $\psi(\infty) = \infty$, $\psi'(\infty) = 1$, then

$$\psi_t(w) := w + t\alpha_0 + t^2 \alpha_1 w^{-1} + ...$$

is the conformal mapping from $\overline{\mathbf{C}} \setminus \{w : |w| \leq t\gamma\}$ into $\overline{\mathbf{C}} \setminus \Omega_t$ with $\psi_t(\infty) = \infty$, $\psi_t'(\infty) = 1$, and so the coefficients of the Laurent expansion of ψ_t can be easily determined from those of ψ.

This may be useful when we want to approximate the evolution operator of some differential problems.

4. Error bounds for truncated Faber series. In this section we want to give an error bound for our approximation (3.6) written in the form

$$y_m := \mathbf{F}_{m-1}(f)(A)\, v, \qquad m \geq 1. \tag{4.1}$$

Assume first that the boundary Γ of Ω is a Jordan curve with bounded *total boundary rotation*, which is defined as

$$V(\Omega) := \int_0^{2\pi} \left|\arg\left(\psi\left(e^{i\gamma t}\right) - \psi\left(e^{i\gamma\vartheta}\right)\right)\right| dt.$$

Let $C_R := \{w : |w| = R\}$. We have the following general result.

PROPOSITION 4.1. *If f is analytic on Ω_R with $\gamma < R < \widehat{R}$ then, for every $\gamma \leq r < R$,*

$$\|f - \mathbf{F}_{m-1}(f)\|_{\Omega_r} \leq \frac{V}{2} M(R) \frac{R}{m} \frac{\left(\frac{r}{R}\right)^m}{1 - \frac{r}{R}}, \tag{4.2}$$

where $V = V(\Omega_r)$ and

$$M(R) := \|f'\|_{\Gamma_R} \left\|\psi'\right\|_{C_R}.$$

Proof. By (3.5) we have that

$$f(z) - \mathbf{F}_{m-1}(f)(z) = \sum_{k=m}^{\infty} a_k F_k(z), \quad m \geq 1. \tag{4.3}$$

By (3.4) we can write

$$a_k = \frac{1}{2\pi R^k} \int_0^{2\pi} f(\psi(R\, e^{i\theta})) e^{-ik\theta} d\theta. \tag{4.4}$$

For $k \geq 1$, changing θ to $\theta + \frac{\pi}{k}$ we easily obtain

$$a_k = -\frac{1}{2\pi R^k}\int_0^{2\pi} e^{-ik\theta} d\theta,$$

and summing with (4.4),

$$a_k = \frac{1}{4\pi R^k}\int_0^{2\pi} \left(f(\psi(R\,e^{i\theta})) - f(\psi(R\,e^{i(\theta+\frac{\pi}{k}}))\right) e^{-ik\theta} d\theta.$$

Now, since

$$\frac{\partial f}{\partial \theta} = f'(\psi(R\,e^{i\theta})\psi'(R\,e^{i\theta})R\,e^{i\theta},$$

we obtain

$$|a_k| \leq \frac{M(R)\pi}{2kR^{k-1}}.$$

Using the well known bound (see e.g. [13])

$$\max_{z\in\Omega_r} |F_m(z)| \leq \frac{V}{\pi} r^m \tag{4.5}$$

and inserting it in (4.3), we get

$$\begin{aligned}
\|f - \mathbf{F}_{m-1}(f)\|_{\Omega_r} &\leq \frac{V}{2} M(R) \sum_{k=m}^{\infty} \frac{1}{k}\frac{r^k}{R^{k-1}} \\
&= \frac{V}{2} M(R) R \sum_{k=m}^{\infty} \frac{1}{k}\left(\frac{r}{R}\right)^k \\
&\leq \frac{V}{2} M(R) \frac{R}{m} \sum_{k=m}^{\infty} \left(\frac{r}{R}\right)^k \\
&= \frac{V}{2} M(R) \frac{R}{m} \frac{\left(\frac{r}{R}\right)^m}{1-\frac{r}{R}}. \qquad \square
\end{aligned}$$

Remark 4.2. *For the quantity* $\|f - \mathbf{F}_{m-1}(f)\|_{\Omega_r}$ *the following simpler bound is also available (see e.g. [13])*

$$\|f - \mathbf{F}_{m-1}(f)\|_{\Omega_r} \leq \frac{V}{\pi}\overline{M}(R)\frac{\left(\frac{r}{R}\right)^m}{1-\frac{r}{R}} \tag{4.6}$$

where

$$\overline{M}(R) := \|f\|_{\Gamma_R},$$

which is easisly obtained using (4.5) and the bound

$$|a_k| \leq \frac{\overline{M}(R)}{R^k},$$

which comes directly from (4.4). Formula (4.6) can be useful when working with f' *to estimate* $M(R)$ *is complicate.*

As previously mentioned, if A is diagonalizable with diagonalization matrix X, and if $\sigma(A) \subseteq \Omega_r$ $(\Omega_\gamma = \Omega)$, for some $\gamma \le r < \widehat{R}$, then for the Euclidean norm of the m-th error vector $e_m := f(A)v - y_m$ the following bound holds (cf.(2.3))

$$\|e_m\|_2 \le cond_2(X)\,\|f - \mathbf{F}_{m-1}(f)\|_{\Omega_r}\,\|v\|_2\,, \qquad m \ge 1, \tag{4.7}$$

where $cond_2(X) = \|X\|_2 \left\|X^{-1}\right\|_2$. In general, a bound of $\|e_m\|_2$ can be obtained as follows, via definition (1.2).

Let $W(A)$ denote the *field of values* (*numerical range*) of A, i.e.

$$W(A) := \left\{ \frac{x^H A x}{x^t x}, x \in \mathbf{C}/\{0\}\,. \right\} \tag{4.8}$$

For the following result see ([32] Th.4.1).

Proposition 4.3. *Under the above assumptions*

$$||(zI - A)^{-1}||_2 \le 1/dist(z, W(A)).$$

□

For simplicity consider tha case (often occurring in practice) that Ω (and so any Ω_r, with $r > \gamma$) is convex, so that $V(\Omega) = 2\pi$.

Proposition 4.4. *Let Ω be convex. Assume that $W(A) \subseteq \Omega_s$, for some $\gamma \le s < \widehat{R}$. Then,*

$$\|e_m\|_2 \le \|v\|_2\,\|f - \mathbf{F}_{m-1}(f)\|_{\Gamma_r}\,\frac{(r+s)}{(r-s)},\ \textit{for any } s < r < \widehat{R}. \tag{4.9}$$

Proof. For any $s < r < \widehat{R}$ it is

$$e_m = \frac{1}{2\pi i}\int_{\Gamma_r} (f(z) - \mathbf{F}_{m-1}(f)(z))(zI - A)^{-1} v\, dz, \quad r > s.$$

Then we get

$$\|e_m\|_2 \le \frac{\|f - \mathbf{F}_{m-1}(f)\|_{\Gamma_r}}{2\pi} \int\limits_{|w|=r} \left|\psi'(w)\right| ||(\psi(w)I - A)^{-1} v||_2 dw.$$

Hence,by Proposition 4.3, we obtain

$$\|e_m\|_2 \le \frac{\|v\|_2\,\|f - \mathbf{F}_{m-1}(f)\|_{\Gamma_r}}{2\pi} \int\limits_{|w|=r} \left| \frac{\psi'(w)}{\psi(w) - u} \right| dw, \tag{4.10}$$

where $u \in \Omega_s$. As well known (cf.[31]), Faber polynomials can be expressed by their generating function, that is we have

$$\frac{w\psi'(w)}{\psi(w) - u} = 1 + \sum_{j=1}^{\infty} F_j(u)\, w^{-j}, \qquad u \in \Omega_s,\ s \ge \gamma,\ |w| > s. \tag{4.11}$$

Using this and

$$\max_{z\in\Omega_s}|F_j(z)|\le 2s^j \tag{4.12}$$

one gets

$$r\left|\frac{\psi^{'}(w)}{\psi(w)-u}\right|\le\frac{(r+s)}{(r-s)},u\in\Omega_s,\quad |w|=r.$$

Then, the thesis follows. □

5. Error bounds for some particular functions. In this section we want to specialize (4.2) or (4.6) for the following four important cases: 1. $f(z)=e^{-z}$, 2. $f(z)=\cos(z)$, 3. $f(z)=e^{-\sqrt{z}}$, 4. $f(z)=\cos(\sqrt{z})$. Throughout this section we assume Ω symmetric with respect to the real axes (since A is real), convex ($V(\Omega)=2\pi$) and strictly contained in the right half plane. It's importat to observe that in the cases 1. and 2. the function involved is analytic in the whole complex plane ($\widehat{R}(f)=\infty$) and, as already mentioned, this property determines the superlinear convergence of the method. On the other hand, cases 3. and 4. involve the square root function that has a singularity in 0, and so they have to be treated with particular attention.

Case 1: $f(z)=e^{-z}$. As well known, this function is related to the Cauchy problem

$$\begin{cases} Au(t)+\frac{du(t)}{dt}=0, & t>0\\ u(0)=v, \end{cases}$$

whose solution is $u(t)=e^{-tA}v$.

Proposition 5.1. *For every $\gamma\le r$ we have*

$$\left\|e^{-\cdot}-\mathbf{F}_{m-1}\left(e^{-\cdot}\right)\right\|_{\Omega_r}\le\frac{8}{m^2}e^{-\psi(-2r)-\frac{m^2}{4r}},\quad m\le 2r, \tag{5.1}$$

$$\left\|e^{-\cdot}-\mathbf{F}_{m-1}\left(e^{-\cdot}\right)\right\|_{\Omega_r}\le\frac{5}{2}e^{-\alpha_0+O(1/m)}\left(\frac{er}{m}\right)^m,\quad m\ge 2r, \tag{5.2}$$

Proof. Let's start considering the case $m\ge 2r$. By our assumptions on Ω and since the exponential function is analytic in the whole complex plane, for each $R>r$ we have

$$\left\|e^{-\cdot}-\mathbf{F}_{m-1}\left(e^{-\cdot}\right)\right\|_{\Omega_r}\le\left\|\psi'\right\|_{C_R}e^{-\psi(-R)}\frac{R}{m}\frac{\left(\frac{r}{R}\right)^m}{1-\frac{r}{R}}, \tag{5.3}$$

because of $\|f'\|_{\Gamma_R}\le\exp(-\psi(-R))$. Setting $R=m$, for $m\ge 2r$ we easily get

$$\left\|e^{-\cdot}-\mathbf{F}_{m-1}\left(e^{-\cdot}\right)\right\|_{\Omega}\le 2\left\|\psi'\right\|_{C_R}e^{-\psi(-m)}\left(\frac{r}{m}\right)^m.$$

Since

$$-\psi(-m)=m-\alpha_0+\frac{\alpha_1}{m}-\frac{\alpha_2}{m^2}+... \tag{5.4}$$

we have

$$\left\|e^{-\cdot}-\mathbf{F}_{m-1}\left(e^{-\cdot}\right)\right\|_{\Omega}\le 2\left\|\psi'\right\|_{C_R}e^{-\alpha_0+O(1/m)}\left(\frac{er}{m}\right)^m.$$

From [20], for ψ' we have the bound

$$\begin{aligned}\left\|\psi'\right\|_{C_R} &\leq 1+\left(\frac{r}{R}\right)^2 \\ &= 1+\left(\frac{r}{m}\right)^2 \leq \frac{5}{4},\end{aligned} \tag{5.5}$$

that leads to (5.2).

For the case $m \leq 2r$, let's start by setting

$$\varepsilon := 1 - r/R, \quad \Rightarrow \quad 0 < \varepsilon < 1 \tag{5.6}$$

Sustituting this in (5.3) we reach

$$\left\|e^{-\cdot} - \mathbf{F}_{m-1}\left(e^{-\cdot}\right)\right\|_{\Omega_r} \leq \left\|\psi'\right\|_{C_R} e^{-\psi\left(\frac{r}{\varepsilon-1}\right)} \frac{1-\varepsilon}{mr\varepsilon}(1-\varepsilon)^m.$$

Using $1-\varepsilon \leq e^{-\varepsilon}$,

$$\left\|e^{-\cdot} - \mathbf{F}_{m-1}\left(e^{-\cdot}\right)\right\|_{\Omega_r} \leq \left\|\psi'\right\|_{C_R} e^{-\psi\left(\frac{r}{\varepsilon-1}\right)} \frac{e^{-m\varepsilon}}{mr\varepsilon}. \tag{5.7}$$

With $\varepsilon := \frac{m}{4r}$, we have that $\varepsilon \leq 1/2$ and $r/(\varepsilon-1) \geq -2r$ for $m \leq 2r$; using these relations in (5.7) it follows that

$$\left\|e^{-\cdot} - \mathbf{F}_{m-1}\left(e^{-\cdot}\right)\right\|_{\Omega_r} \leq \frac{4}{m^2}\left\|\psi'\right\|_{C_R} e^{-\psi(-2r)-\frac{m^2}{4r}},$$

and the thesis is reached because by (5.5)

$$\left\|\psi'\right\|_{C_R} \leq 2. \qquad \square \tag{5.8}$$

Case 2: $f(z) = \cos(z)$. For the following Proposition let us make the further hypotesis that Ω has a vertical axis.

PROPOSITION 5.2. *For every $\gamma \leq r$ we have*

$$\|\cos - \mathbf{F}_{m-1}(\cos)\|_{\Omega_r} \leq \frac{8}{m^2}\cosh(\operatorname{Im}(\psi(2ri))\, e^{-\frac{m^2}{4r}}, \quad m \leq 2r, \tag{5.9}$$

$$\|\cos - \mathbf{F}_{m-1}(\cos)\|_{\Omega_r} \leq \frac{5}{2}e^{O(1/m)}\left(\frac{er}{m}\right)^m, \quad m \geq 2r, \tag{5.10}$$

Proof. Let' start with the case $m \geq 2r$. Using (4.2), for each $R > r$ we find

$$\|\cos - \mathbf{F}_{m-1}(\cos)\|_{\Omega_r} \leq \|\sin\|_{\Gamma_R}\left\|\psi'\right\|_{C_R} \frac{R}{m}\frac{\left(\frac{r}{R}\right)^m}{1-\frac{r}{R}}.$$

In order to estimate $\|\sin\|_{\Gamma_R}$, writing $z = x + iy$ we have

$$\sin z = \sin x \cosh y + i \sinh y \cos x$$

and thus

$$|\sin z| = \sqrt{1-\cos^2(x)+\sinh^2(y)}.$$

Using this formula and all the hypotesis on Ω, have

$$\|\sin\|_{\Gamma_R} \leq \cosh\left(\operatorname{Im}\psi(iR)\right).$$

As in the previous Proposition we define $R = m$ and for $m \geq 2r$ we find

$$\|\cos - \mathbf{F}_{m-1}(\cos)\|_{\Omega_r} \leq 2\left\|\psi'\right\|_{C_R} \cosh\left(\operatorname{Im}\psi(im)\right)\left(\frac{r}{m}\right)^m.$$

Now,

$$\operatorname{Im}\psi(im) = \operatorname{Im}\left(im + \alpha_0 - \frac{i\alpha_1}{m} - \frac{\alpha_2}{m^2} + ...\right) = m - \frac{\alpha_1}{m} + O(1/m^3), \tag{5.11}$$

that leads to

$$\cosh\left(\operatorname{Im}\psi(im)\right) \leq e^{\operatorname{Im}\psi(im)} \leq e^{m+O(1/m)}.$$

By (5.5) we finally obtain (5.10).

For $m \leq 2r$, we can proceed as in the previous Proposition getting

$$\|\cos - \mathbf{F}_{m-1}(\cos)\|_{\Omega_r} \leq \frac{4}{m^2}\left\|\psi'\right\|_{C_R} \cosh\left(\operatorname{Im}\left(\psi\left(\frac{ir}{1-\varepsilon}\right)\right)\right) e^{-\frac{m^2}{4r}}.$$

The thesis follows straightfully from (5.8) and

$$\frac{r}{1-\varepsilon} \leq 2r.$$

□

Case 3: $f(z) = e^{-\sqrt{z}}$. As said before, in this case the function involved is not analytic in the whole complex plane because the square root function is singular in 0. As consequence there will be not superlinear convergence. By the theory of Faber polynomials, for a general function f, it is known that

$$\overline{\lim}_{m\to\infty} \|f - \mathbf{F}_{m-1}(f)\|_{\Omega_r}^{1/(m-1)} = \frac{r}{\widehat{R}(f)}, \tag{5.12}$$

where $\widehat{R}(f)$ is defined in Sect. 3 (cf. (3.9)). Therefore, for this case our aim is to find out a bound whose asymptotical behaviour is described by (5.12).

We must specify that here we consider only the branch of the square root such that $\sqrt{1} = 1$. Namely, on the basis of definition (1.2) we set

$$A^{1/2}v = \frac{1}{2\pi i}\int_\Gamma z^{1/2}(zI - A)^{-1}v\ dz, \tag{5.13}$$

With this assumption the square root can be considered analytic in all regions not containing 0 and ∞.

We recall that $u(t) = e^{-tA^{1/2}}v$ solves the boundary value problem

$$\begin{cases} Au(t) - \frac{d^2u(t)}{dt^2} = 0, \quad t > 0, \\ u(0) = v, \quad u(\infty) = 0. \end{cases}$$

PROPOSITION 5.3. *For every $\gamma \le r$ and $m \ge 2$, it is*

$$\left\| e^{-\sqrt{\cdot}} - \mathbf{F}_{m-1}\left(e^{-\sqrt{\cdot}}\right)\right\|_{\Omega_r} \le \frac{K}{\sqrt{m}} e^{-O(1/\sqrt{m})} \left(\frac{r}{\widehat{R}}\right)^m \tag{5.14}$$

where K is a constant depending on Ω_r and his position with respect to the point 0.

Proof. By (4.2), for $\gamma < R < \widehat{R}$ we easily get

$$\begin{aligned}\left\| e^{-\sqrt{\cdot}} - \mathbf{F}_{m-1}\left(e^{-\sqrt{\cdot}}\right)\right\|_{\Omega_r} &\le \|\psi'\|_{C_R} \frac{1}{2} \max_{z\in\Gamma_R} \left|\frac{e^{-\sqrt{z}}}{\sqrt{z}}\right| \frac{R}{m} \frac{\left(\frac{r}{R}\right)^m}{1-\frac{r}{R}},\\ &= \|\psi'\|_{C_R} \frac{1}{2} \frac{e^{-\sqrt{\psi(-R)}}}{\sqrt{\psi(-R)}} \frac{R}{m} \frac{\left(\frac{r}{R}\right)^m}{1-\frac{r}{R}}.\end{aligned} \tag{5.15}$$

For $m \ge 2$ we define

$$R = R(m) := \widehat{R} - \frac{\varepsilon}{m}, \tag{5.16}$$

where $\varepsilon := \widehat{R} - \gamma$. Thus $R(m) \to \widehat{R}$ for $m \to \infty$. Since $m \ge 2$, we have

$$1 - \frac{r}{R(m)} \le \frac{\widehat{R}+r}{\widehat{R}-r}, \quad \text{and} \quad \frac{R(m)}{m} = \frac{\widehat{R}}{m} - \frac{\varepsilon}{m^2} = O(1/m). \tag{5.17}$$

Regarding $\psi(-R(m))$, using (5.16) after some computations we obtain the relation

$$\psi(-R(m)) = \psi(-\widehat{R}) + O(1/m) = O(1/m), \tag{5.18}$$

because $\psi(-R^*) = 0$. Hence we have that

$$\frac{e^{-\sqrt{\psi(-R)}}}{\sqrt{\psi(-R)}} = \frac{e^{-O(1/\sqrt{m})}}{O(1/\sqrt{m})}. \tag{5.19}$$

By (5.16), since $m \ge 2$ we also have

$$\begin{aligned}\left(\frac{r}{R(m)}\right)^m &= \left(\frac{r}{\widehat{R}}\right)^m \left(\frac{1}{1-\frac{\varepsilon}{\widehat{R}m}}\right)^m\\ &\le \left(\frac{r}{\widehat{R}}\right)^m \left(\frac{2\widehat{R}}{2\widehat{R}-\varepsilon}\right)^2 = \left(\frac{r}{\widehat{R}}\right)^m \left(\frac{2\widehat{R}}{\widehat{R}+r}\right)^2\end{aligned} \tag{5.20}$$

and

$$\begin{aligned}\|\psi'\|_{C_R} &\le 1 + \left(\frac{r}{R}\right)^2\\ &= 1 + \frac{r^2}{\left(\widehat{R}-\frac{\varepsilon}{m}\right)^2} \le 1 + \frac{4r^2}{\varepsilon^2}.\end{aligned} \tag{5.21}$$

Joining all previous results in (5.15) we get

$$\left\| e^{-\sqrt{\cdot}} - \mathbf{F}_{m-1}\left(e^{-\sqrt{\cdot}}\right)\right\|_{\Omega} \le$$
$$\tfrac{1}{2}\left(1+\tfrac{4r^2}{(\widehat{R}-r)^2}\right) \tfrac{\widehat{R}+r}{\widehat{R}-r} \left(\tfrac{2\widehat{R}}{\widehat{R}+r}\right)^2 \tfrac{C}{\sqrt{m}} e^{-O(1/\sqrt{m})} \left(\tfrac{r}{\widehat{R}}\right)^m$$

which proves the thesis that satisfies the property (5.12). $\square$

Case 4: $f(z) = \cos(\sqrt{z})$. Let's start making some considerations. As already said, the square root function is not single valued. In fact it is two valued, having a branch for which $\sqrt{1} = 1$ and another for which $\sqrt{1} = -1$. However, since we are working with the cosinus, the composite function is single valued. Moreover, by expanding we get

$$\cos\sqrt{z} = 1 - \frac{z}{2!} + \frac{z^2}{4!} - ... \tag{5.22}$$

Since (5.22) converges for each $z \in \mathbf{C}$, we have that $\cos\sqrt{z}$ is analytic in the whole complex plane.

Note that this function is related to the Cauchy problem

$$\begin{cases} Au(t) - \frac{d^2u(t)}{dt^2} = 0, \quad t > 0, \\ u(0) = v, \quad \frac{du}{dt}(0) = 0, \end{cases}$$

whose solution is $u(t) = \cos(tA^{1/2})v$.

Also in this case, for the following Proposition we make the further hypotesis that Ω has a vertical axis.

PROPOSITION 5.4. *For $m \geq 2r$,*

$$\left\|\cos(\sqrt{\cdot}) - \mathbf{F}_{m-1}\left(\cos(\sqrt{\cdot})\right)\right\|_{\Omega_r} \leq 4e^{c_1\sqrt{m} + c_2\frac{\alpha_0}{\sqrt{m}} + O\left(1/m^{3/2}\right)}\left(\frac{r}{m}\right)^m. \tag{5.23}$$

where c_1 and c_2 are positive constants.

Proof. For this case, instead of (4.2) it is much more convenient to use the estimate (4.6), which leads to

$$\left\|\cos(\sqrt{\cdot}) - \mathbf{F}_{m-1}\left(\cos(\sqrt{\cdot})\right)\right\|_{\Omega} \leq 2\max_{z\in\Gamma_R}\left|\cos\left(\sqrt{z}\right)\right|\frac{\left(\frac{r}{R}\right)^m}{1-\frac{r}{R}}, \tag{5.24}$$

for $r < R < \infty$. Writing $z = x + iy$ and defining

$$a := \sqrt{\frac{1}{2}\sqrt{x^2+y^2} + \frac{1}{2}x}, \quad b := \sqrt{\frac{1}{2}\sqrt{x^2+y^2} - \frac{1}{2}x},$$

we have

$$\begin{aligned} \left|\cos\left(\sqrt{x+iy}\right)\right| &= \sqrt{\cos^2(a)\cosh^2(b) + \sin^2(a)\sinh^2(b)} \\ &\leq \sqrt{\cosh^2(b) + \sinh^2(b)} \\ &\leq \cosh(b) + \sinh(b) = e^b. \end{aligned}$$

The function e^b goes to $+\infty$ as $x \to -\infty$ or $y \to \infty$, so that we can put $x := \psi(-R)$ and $y := \operatorname{Im}\psi(iR)$, obtaining

$$\max_{z\in\Gamma_R}\left|\cos\left(\sqrt{z}\right)\right| \leq e^{\frac{1}{\sqrt{2}}\sqrt{\sqrt{(\psi(-R))^2 + (\operatorname{Im}\psi(iR))^2} - \psi(-R)}}.$$

Now, setting $R = m$ as in Propositions 5.1 and 5.2, and using formulas (5.4) and (5.11), from the above relation, as $m \to \infty$ we get

$$
\begin{aligned}
\max_{z \in \Gamma_R} \left|\cos\left(\sqrt{z}\right)\right| &\leq e^{\frac{1}{\sqrt{2}}\sqrt{\sqrt{2m^2-2m\alpha_0+\alpha_0^2-\frac{2\alpha_0\alpha_1}{m}+O(1/m^2)}+m-\alpha_0+\frac{\alpha_1}{m}+O(1/m^2)}} \\
&= e^{\frac{1}{\sqrt{2}}\sqrt{\left(\sqrt{2}+1\right)m+\left(1-\frac{\sqrt{2}}{2}\right)\alpha_0+\left(\frac{\sqrt{2}}{8}\alpha_0^2+1\right)\frac{1}{m}+O(1/m^2)}} \\
&= e^{\frac{\sqrt{\sqrt{2}+1}}{\sqrt{2}}\sqrt{m}+\frac{1}{2\sqrt{2}}\left(1-\frac{\sqrt{2}}{2}\right)\left(\frac{1}{\sqrt{\sqrt{2}+1}}\right)\alpha_0\frac{1}{\sqrt{m}}+O\left(\frac{1}{m^{3/2}}\right)}
\end{aligned}
$$

which proves the thesis. $\square$

For various cases of interest, like those considered for instance in [17], [25], [26], the previous general bounds can be specialized, taking into account the particular structure of Ω. Accordingly estimates of the error e_m will follow from (4.7) or using Proposition 4.3 with a suitable choice of r in (4.9), as we show, as an example, here below.

PROPOSITION 5.5. *Assume that $W(A) \subseteq \Omega_s$, for some $\gamma \leq s$ and that there is are positive constants C and c such that for every $r \geq s$*

$$\left\|f - \mathbf{F}_{m-1}\left(f\right)\right\|_{\Omega_r} \leq C\left(\frac{cr}{m}\right)^m \tag{5.25}$$

then

$$\left\|e_m\right\|_2 \leq 2csC\left(\frac{cs}{m-1}\right)^{m-1}\left\|v\right\|_2. \tag{5.26}$$

Proof. The result follows easily by application of Proposition 4.3 , taking in (4.9) $r = sm/(m-1)$. $\square$

6. Numerical implementation. Until this moment for the definition of the methods we supposed to work with a certain compact subset Ω containing $\sigma\left(A\right)$. Actually, we observed that condition $\sigma\left(A\right) \subseteq \Omega$ is not essential for the convergence (cf.(4.7)). Moreover, by condition (2.3) the rate of convergence is clearly as faster as better the compact Ω approximates the convex hull of the spectrum, and in the more general case, as better $\Omega \in \mathbf{M}$ approximates the smallest connected compact Ω_{opt} such that $\sigma\left(A\right) \subseteq \Omega_{opt}$.

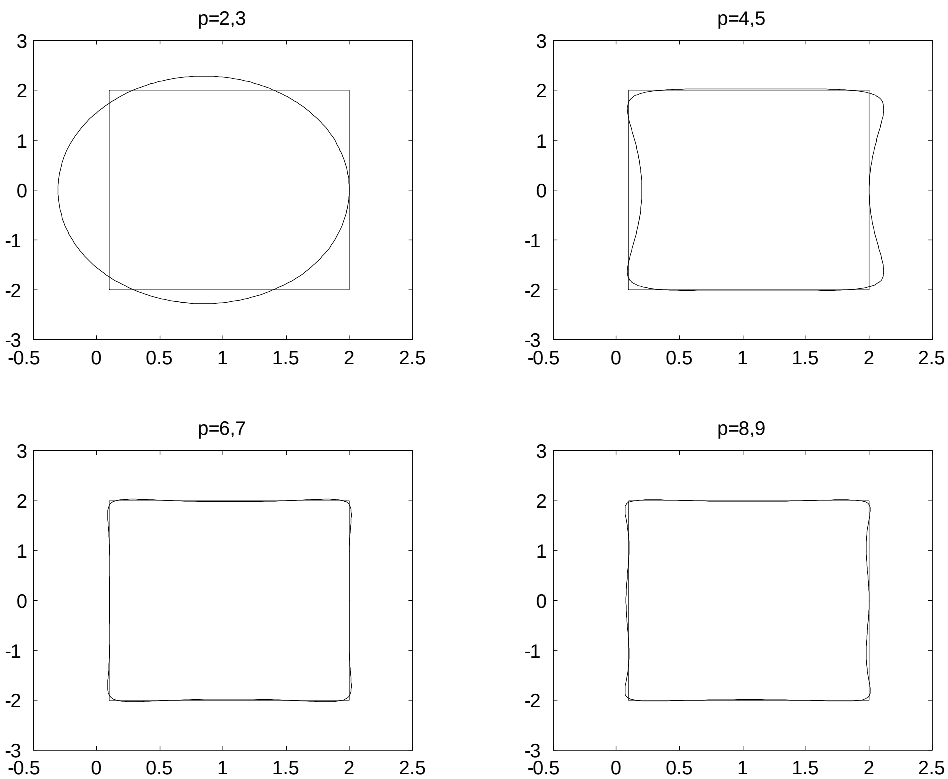
In practice, the simplest way to build Ω consists of using an eigenvalues- estimating method to yield a certain number of estimates for $\sigma\left(A\right)$ and then considering Ω as the compact whose boundary is the polygon obtained joining the marginal points of the estimates set (cf. [24], [33]). Since we consider A real, $\sigma\left(A\right)$ is symmetric with respect to the real axis and then we can also consider a polygon of this type. Nevertheless we must point out that if the function f is not analytic in the whole complex plane, in some cases it could be necessary to approximate very well $\sigma\left(A\right)$. In fact if the $\sigma\left(A\right)$ is very closed to a singular point of f, it could happen that the eigenvalue estimating phase leads to a compact Ω containing such singular point, determining the failure of the method. In a such case we can proceed using an eigenvalue method very accurate (for example the Arnoldi algorithm made run for a large number of iteration), or the method proposed in [24] based on the Arnoldi algorithm to estimate the field of values of A^{-1}. If f is analytic in the whole complex plane, even a not very efficient eigenvalue method yields acceptable results.

In order to determine the Laurent expansion of ψ, we can proceed using the scheme proposed in [33], based on the resolution of the parameters problem relative to the Schwarz-Christoffel transformation associated to the mapping ψ, for which we refer to [36]. Obviously,only a finite number of coefficients of this expansion can be determined numerically, and so, fixing a priori this number, instead of ψ we obtain the finite expansion of a conformal mapping

$$\psi^* : \overline{\mathbf{C}} \backslash \{w : |w| \leq \gamma^*\} \to \overline{\mathbf{C}} \backslash \Omega^*,$$

which represents an approximation of ψ, such that $\gamma^* \approx \gamma$ and $\Omega^* \approx \Omega$.

Theoretically, the optimal situation consists of working directly with Ω_{opt}, that is building the method on this compact subset. So, in general, working with ψ^* produces the effect of making further worse the optimal situation, already weakened by the fact that we are working on the compact Ω determined by an estimates set instead of $\sigma(A)$. On the other hand, from the computational point of view, working on Ω^* (with the mapping ψ^*) is clearly an advantage because in this way formula (3.2) is a recurrence with a fixed finite number of terms. In the particular case that we compute the only first two coefficients of the Laurent expansion of ψ, that is c_0 e c_1,we work with scaled and translated Chebychev polynomials (cf.[16], [22], [23]).



Accordingly with what sayd above, if it is necessary to give a good estimate of $\sigma(A)$, it is important to compute a certain number of the leading coefficients of ψ.In the figure above we consider four approximations ψ^* of the conformal mapping relative to the compact $\Omega = [0.1, 2] \times [-2i, 2i]$ whose associated mapping ψ has an infinite Laurent expansion with $\alpha_{2n+1} = 0$ for each $n \geq 1$. In figure we indicate with p the number of its computed leading coefficients, so that

$$\psi^{*}(w) = w + c_0^* + c_1^* w^{-1} + ... + c_p^* w^{-p}.$$

We can immediately observe that the good quality of the approximation of Ω by means of Ω^* improves as p increases. In particular, if $p = 2, 3$, the approximation is given by an ellipse that contains the point 0. Hence, if this point is a singularity of the function considered, the method fails whereas for $p > 3$ the approximation leads to a convergent method.

A further consideration has to be made when A is symmetric or skew-symmetric: in this situation, if we can achieve an interval as approximation of the smallest interval containing $\sigma(A)$ (this possibility depends on the algorithm that we use for estimating the eigenvalues of A) the associated conformal mapping ψ has a three terms expansion, it can be computed exactly and we reach anyhow methods based on Chebychev polynomials.

Concerning the method of the truncated Faber series, in order to define the iteration parameters in (3.10) it is also necessary to compute the Faber coefficients (3.4) using some numerical integration rule. In particular, we we use a k-point trapezium rule, evaluating as many of the a_j as we require. About the choice of $R > \gamma$, for a generic function $f(z)$ it is necessary to avoid that the compact Ω_R contains any singularity of $f(z)$. The value $R = \gamma$ is also acceptable when the mapping ψ can be extended continuously to the boundary $|w| = \gamma$ [13], as for example in the case of the polygon.

In summary the preliminary phases we need for the implementation of our schemes are:

1. construction of the polygon Ω containing $\sigma(A)$;
2. evaluation of the first p coefficients of the Laurent series expansion of the mapping ψ defined by (3.3);

If, to build Ω, we use an eigenvalue estimating algorithm, such algorithm must be suitable for this purpose. The power method, used in [23] or the Arnoldi method used in [33], represent possible choices. Obviously in this phase no approximation for $f(A)v$ is achieved but only information on A, and so we can say it produces a certain "delay" for the computation of $f(A)v$, which does not regard Krylov type methods. Nevertheless this information can be re-used every time we want to compute $f(A)v$ with different vectors v, for example implementing the integrators discussed in [14] and [18]. The cost for the computation of the p-truncated expansion of ψ is independent of the order of A, and, if Ω is a polygon, it is proportional to the number of its vertices.

7. Numerical experiments. In the example that follows we illustrate the behavior of the method, making a comparison with the Krylov methods based on the Arnoldi and Lanczos algorithms (see e.g. [30]). Let us consider the differential operator

$$L = \Delta - \tau_1 \frac{\partial}{\partial x} - \tau_2 \frac{\partial}{\partial y}, \qquad \tau_1, \tau_2 \in \mathbf{R}. \tag{7.1}$$

Discretizing using central differences on the cube $(0,1) \times (0,1) \times (0,1)$ with uniform meshsize $h = 1/(n+1)$ along each direction, a nonsymmetric matrix $\overline{A}$ of order $N = n^3$ with particular block structure is obtained. It can be represented in the following way,

$$\overline{A} := \frac{1}{h^2}\left\{ I_n \otimes (I_n \otimes C_1) + [B \otimes I_n + I_n \otimes C_2] \otimes I_n \right\},$$

where B is defined as

$$B := \begin{bmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & 1 & \ddots & \ddots \\ & & \ddots & \ddots \end{bmatrix},$$

I_n is the n-order matrix identity, and, by setting $\mu_i := \tau_i\,(h/2)$,

$$C_i := \begin{bmatrix} -2 & 1-\mu_i & & \\ 1+\mu_i & -2 & 1-\mu_i & \\ & 1+\mu_i & \ddots & \ddots \\ & & \ddots & \ddots \end{bmatrix}, \qquad i = 1, 2.$$

Defining $A = h^2\overline{A}$ and

$$\lambda_n := \cos\left(\frac{\pi}{n+1}\right)\left(\sqrt{1-\mu_1^2} + \sqrt{1-\mu_2^2} + 1\right),$$

the spectrum of A is contained in the rectangle

$$R = [-6 - 2\operatorname{Re}\lambda_n, -6 + 2\operatorname{Re}\lambda_n] \times [-2i\operatorname{Im}\lambda_n, 2i\operatorname{Im}\lambda_n],$$

that we directly use to build the method (i.e. we define $\Omega := R$).

In the table below, *err* is the final $\|e_m\|_2$ achieved, p (as in Sect.6) indicates the number of the computed leading Laurent coefficients of ψ, *nit* is the number of iteration of the methods employed and *nsp* is the corresponding number of scalar products performed (taking into account of the sparsity pattern of A). In all tests, $N = 3375$.

			Faber			Arnoldi		Lanczos		
μ_1	μ_2	*err*	p	*nit*	*nsp*	*nit*	*nsp*	*nit*	*nsp*	$f(z)$
2	2	10^{-8}	5	31	198	28	590	31	471	e^z
3	5	10^{-8}	5	40	257	37	947	38	577	
5	10	10^{-8}	5	56	363	52	1721	54	820	
1	2	10^{-7}	5	31	170	26	498	31	413	$\cos z$
2	3	10^{-7}	5	36	231	32	739	34	516	
3	4	10^{-7}	5	41	264	38	991	86	1307	
2	2	10^{-7}	4-5	59	382	50	1605	60	912	$e^{-\sqrt{z}}$
			7-9	56	363					
3	2	10^{-7}	3	104	679	56	1965	63	957	
			4-5	63	409					
			7-9	61	396					
4	3	10^{-7}	3	183	1201	67	2720	78	1185	
			4-5	73	475					
			7-9	71	462					
3	3	10^{-9}	5	12	72	10	121	11	167	$\cos\sqrt{z}$
8	9	10^{-9}	5	14	85	13	176	13	197	
15	25	10^{-9}	5	18	112	16	241	16	243	

REMARK 7.1. *For the computation of the Laurent coefficients of ψ we employed the software SC Matlab Toolbox, written by T.A.Driscoll at M.I.T. in 1995.*

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