A convergence analysis for the shift-and-invert Krylov subspace method

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Abstract

Time integration methods for stiff systems of ordinary differential equations often involve the product of a matrix function $f(A)$ and some vector v. The matrix A typically arises from a spatial discretization of a partial differential equation. The refinement of the space grid therefore results in a very large norm of the discretization matrix A. For the approximation of $f(A)v$ in the shift-and-invert Krylov subspace, we prove a convergence rate that does not depend on this norm. The efficiency of the shift-and-invert Krylov method in comparison to the standard Krylov approximation is illustrated by several numerical experiments.

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matrix functions, φ-functions, rational Krylov subspace method, rational approximation
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1. Introduction

The spatial discretization of a semilinear partial differential equation usually leads to a system of ordinary differential equations of the form

$$u'(t) = Au(t) + g\big(t, u(t)\big)\,, \quad u(0) = u_0 \tag{1}$$

with a large and sparse discretization matrix $A \in \mathbb{C}^{N\times N}$, whose dimension N depends on the refinement of the grid in space. Typically, the semilinear

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problem (1) consists of a nonlinear non-stiff part $g\big(t, u(t)\big)$ and a linear stiff part $Au(t)$. For an inner product $(\cdot\,,\cdot)$ on $\mathbb{C}^N$ and its associated norm $\|\cdot\|$, stiffness might be characterized by the fact that the matrix A can have an arbitrarily large field-of-values

$$W(A) := \{(Ax, x) \,:\, x \in \mathbb{C}^N, \|x\| = 1\}$$

in the left complex half-plane

$$\mathbb{C}_0^- := \{z \in \mathbb{C} \,:\, \mathrm{Re}(z) \leq 0\}$$

and that the norm of A grows for finer and finer space discretizations. Such matrices we will call "stiff" in the following.

Exponential integrators constitute a promising tool for the numerical solution of (1). The fundamental idea behind this class of integrators is to solve the linear part exactly by the matrix exponential $e^{\tau A}$ times the initial data u_0 and to approximate the remaining nonlinear part in a suitable way. A detailed review of exponential integrators can be found in [14].

The simplest exponential integrator is obtained by approximating the nonlinearity $g\big(t, u(t)\big)$ in (1) by the constant $g(0, u_0)$ which yields the exponential Euler method

$$u(\tau) \approx e^{\tau A} u_0 + \tau \varphi_1(\tau A) g(0, u_0) \quad \text{with} \quad \varphi_1(z) = \frac{e^z - 1}{z}\,.$$

In general, the time integration schemes of exponential integrators require the computation of the so-called φ-functions of the matrix τA. These functions are defined as

$$\varphi_\ell(z) = \int_0^1 e^{(1-s)z} \frac{s^{\ell-1}}{(\ell-1)!}\, ds\,, \quad \ell \geq 1\,.$$

An alternative representation is given by

$$\varphi_\ell(z) = \frac{e^z - t_{\ell-1}(z)}{z^\ell}\,, \quad t_{\ell-1}(z) = \sum_{k=0}^{\ell-1} \frac{z^k}{k!}\,. \tag{2}$$

For the successful application of exponential integrators, the efficient approximation of $\varphi_\ell(\tau A)$ times some vector v is of great importance. Since the temporal convergence of these integrators is independent of $\|A\|$ and since a large norm of A does not necessitate a restriction of the admissible time step size, we are interested in an approximation of $\varphi_\ell(\tau A)v$ that preserves these favorable properties. More precisely, we would like to approximate the matrix functions appearing in exponential integrators independent of the refinement of the spatial grid.

Krylov subspace methods represent a possible tool for the approximation of a general matrix function $f(A)$ times a vector v. Using the standard Krylov method, we approximate $f(A)v$ in the subspace

$$\mathcal{K}_m(A, v) = \text{span}\{v, Av, \ldots, A^{m-1}v\}\,.$$

For matrices A with a large norm, it is known that a substantial error reduction usually starts only after many iteration steps, e.g. [13]. The situation is different for rational Krylov subspace techniques which have been recently studied by a number of papers, see e.g. [2, 4, 6, 10, 11, 15–21, 23]. Here, we will focus on the shift-and-invert Krylov subspace

$$\mathcal{K}_m\big((\gamma I - A)^{-1}, v\big) = \text{span}\{v, (\gamma I - A)^{-1}v, \ldots, (\gamma I - A)^{-m+1}v\}\,.$$

The subsequent example demonstrates the beneficial properties of the rational method: The rational Krylov subspace iteration for the approximation of a matrix function $f(A)$ times v converges independently of $\|A\|$, whereas the standard Krylov subspace iteration does not. To illustrate this fact, we consider the one-dimensional heat equation $U' = \Delta U$, $U(0) = x(1-x)$ with homogeneous Dirichlet boundary conditions on $(0, 1)$. The discretization by finite differences with N grid points results in a system of ordinary differential equations

$$u'(t) = Au(t)\,, \quad u(0) = u_0 \in \mathbb{R}^N$$

with the discretization matrix

$$A = (N+1)^2 \text{tridiag}(1, -2, 1) \in \mathbb{R}^{N \times N}$$

having a field-of-values on the negative real axis and a matrix norm (induced by the discrete L^2-norm) that grows like N^2. The exact solution $u(\tau) = e^{\tau A}u_0$ is for $\tau = 0.05$ approximated in the standard and in the shift-and-invert Krylov subspace with the shift $\gamma = 1$. The associated error curves are depicted in Figure 1. We see that the convergence behavior of the standard Krylov approximation is strongly related to the number N of discretization points. The finer the discretization the slower is the error reduction. By contrast, the rational method achieves independently of N a high accuracy in just a few iteration steps.

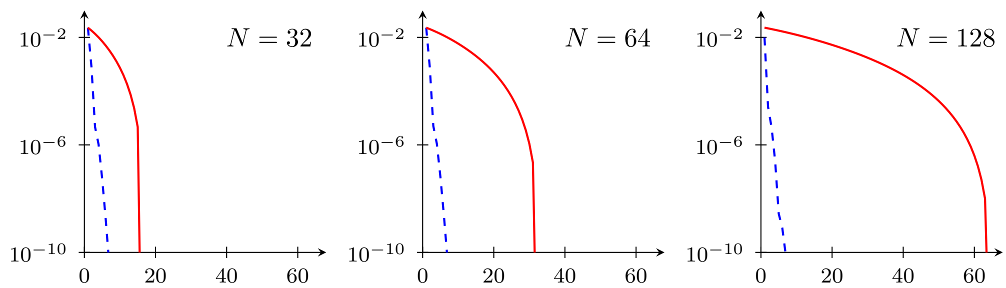

Figure 1: Comparison of the standard (red solid lines) and the shift-and-invert (blue dashed lines) Krylov method for different refinements of the spatial grid. The error is plotted against the dimension of the Krylov subspace used for the approximation of $e^{\tau A}u_0$.

The main goal of this paper is to explain this observation. For stiff matrices A with an arbitrarily large field-of-values in the left complex half-plane and a special class of functions, including the φ-functions, we prove that $f(A)v$ can be approximated grid-independent, that is independent of $\|A\|$, in the shift-and-invert Krylov subspace $\mathcal{K}_m\big((\gamma I - A)^{-1}, v\big)$. For operators $\mathcal{A}$ generating a strongly continuous semigroup on some Hilbert space and operator functions $f(\mathcal{A})$, this has been shown by Grimm in [8] with the help of a suitable functional calculus and a rather complicated modulus of smoothness. Here, we follow a simpler way involving the standard modulus of continuity which is easier to handle. By transforming the left half-plane to the unit disk, we obtain sublinear error bounds that depend on the smoothness of a transformed version of the function f on the boundary of this disk. These bounds explain the grid-independent convergence.

The paper is organized as follows. After the introduction in this section, we summarize the most important properties of the shift-and-invert Krylov subspace method in Section 2. In Section 3, we transform the rational approximation problem to a trigonometric one and we establish error bounds for the special case of the φ-functions in Section 4. Our findings are illustrated by some numerical experiments in Section 5. Finally, we close with a short conclusion.

2. The shift-and-invert Krylov subspace method

The rational Krylov subspace method was first proposed by Ruhe [22] for large and sparse eigenvalue problems. Recently, the method is used to approximate matrix functions applied to some vector. The approximation is based on rational functions of the matrix A with either the same or different poles distinct from the spectrum of A. The shift-and-invert Krylov subspace

$$\mathcal{Q}_m(A, v) := \mathcal{K}_m\big((\gamma I - A)^{-1}, v\big)$$

considered here has a multiple pole at γ. For a shift $\gamma > 0$ and a stiff matrix A with a field-of-values in the left complex half-plane, this inverse is well defined. Instead of $(\gamma I - A)^{-1}$, we will sometimes write $\frac{1}{\gamma - A}$ in the spirit of matrix functions in order to improve readability. The subspaces $\mathcal{Q}_m(A, v)$ form a nested sequence

$$\mathcal{Q}_1(A, v) \subsetneq \mathcal{Q}_2(A, v) \subsetneq \ldots \mathcal{Q}_\mu(A, v) = \mathcal{Q}_{\mu+1}(A, v) = \ldots$$

until some invariance index μ is reached. Since

$$\dim\big(\mathcal{Q}_m(A, v)\big) = \dim\big((\gamma I - A)^{-m+1}\mathcal{K}_m(A, v)\big) = \dim\big(\mathcal{K}_m(A, v)\big)\,,$$

the invariance index μ of $\mathcal{Q}_m(A, v)$ is identical with the invariance index of the standard Krylov subspace $\mathcal{K}_m(A, v)$. The following alternative representation will be useful for later purposes.

Lemma 1. *We have*

$$\begin{aligned}\mathcal{Q}_m(A, v) &= \operatorname{span}\left\{v, \frac{1}{\gamma - A}\, v, \ldots, \frac{1}{(\gamma - A)^{m-1}}\, v\right\} \\ &= \operatorname{span}\left\{v, \frac{\gamma + A}{\gamma - A}\, v, \ldots, \left(\frac{\gamma + A}{\gamma - A}\right)^{m-1} v\right\}.\end{aligned}$$

Proof. We denote by $\mathcal{P}_{m-1}$ the space of all polynomials with degree at most $m-1$. The statement follows from the fact that for any coefficients a_k, $k = 0, \ldots, m-1$, we can find a polynomial $p_{m-1} \in \mathcal{P}_{m-1}$ with

$$\sum_{k=0}^{m-1} a_k \frac{1}{(\gamma - z)^k} = \frac{p_{m-1}(z)}{(\gamma - z)^{m-1}}\,, \quad z \in \mathbb{C}\backslash\{\gamma\}\,. \tag{3}$$

Conversely, by partial fraction decomposition there exist for every $p_{m-1} \in \mathcal{P}_{m-1}$ coefficients a_k, $k = 0, \ldots, m-1$, such that (3) holds true. □

For a matrix function $f(A)$ and some vector v, we have $f(A)v \in \mathcal{Q}_\mu(A,v)$, but the invariance index μ for which this happens is usually quite large. In this case, we compute a suitable approximation to $f(A)v$ in $\mathcal{Q}_m(A,v)$ with $m < \mu$ by using an orthogonal projection onto the shift-and-invert Krylov subspace. Therefore, we first compute an orthonormal basis $V_m = [v_1\ v_2 \cdots v_m] \in \mathbb{C}^{N\times m}$ of $\mathcal{Q}_m(A,v)$ by the rational Arnoldi process whose pseudocode is given in Algorithm 1. When an orthonormal basis is known, the orthogonal projector onto $\mathcal{Q}_m(A,v)$ is given by $V_mV_m^+$, where V_m^+ is the Moore-Penrose pseudoinverse with respect to the chosen inner product $(\cdot\,,\cdot)$.

Algorithm 1: Rational Arnoldi algorithm

```
Data: matrix A ∈ C^{N×N}, vector v ∈ C^N, shift γ > 0
v_1 = v/‖v‖
for m = 1, 2, ... do
    for j = 1, 2, ..., m do
        h_{j,m} = ((γI − A)^{-1} v_m, v_j)
    end
    ṽ_{m+1} = (γI − A)^{-1} v_m − Σ_{j=1}^{m} h_{j,m} v_j
    h_{m+1,m} = ‖ṽ_{m+1}‖
    v_{m+1} = ṽ_{m+1}/h_{m+1,m}
end
```

Definition 2. *For a function f analytic in $\mathbb{C}_0^-$, a matrix $A \in \mathbb{C}^{N\times N}$ with $W(A) \subseteq \mathbb{C}_0^-$, and the orthogonal projector $P_m = V_mV_m^+$ onto $\mathcal{Q}_m(A,v)$, the shift-and-invert Krylov subspace approximation is defined as*

$$f(A)v \approx f(A_m)v = f(P_mAP_m)v = V_mf(V_m^+AV_m)V_m^+v = \|v\|V_mf(S_m)e_1\,,$$

where the matrix $A_m = P_mAP_m \in \mathbb{C}^{N\times N}$ can be seen as a restriction and $S_m = V_m^+AV_m \in \mathbb{C}^{m\times m}$ as a compression of A to $\mathcal{Q}_m(A,v)$.

Using the Krylov approximation $\|v\|V_mf(S_m)e_1$ for $f(A)v$, the original problem of dimension N is reduced to a smaller dimension $m \ll N$. The function f now has to be evaluated for a small $m\times m$ - matrix only. This can be done by standard algorithms for dense matrices (cf. [12]).

The next lemma regarding the exactness of the shift-and-invert Krylov subspace approximation for specific rational functions turns out to be very useful in order to establish error bounds. A proof can be found in [3].

Lemma 3. *Let r be a function of the form $r(z) = p_{m-1}(z)/(\gamma - z)^{m-1}$ with $p_{m-1} \in \mathcal{P}_{m-1}$. Then the approximation of $r(A)v$ in $\mathcal{Q}_m(A, v)$ fulfills*

$$r(A)v = r(A_m)v = \|v\| V_m r(S_m) e_1 \,.$$

With the help of Lemma 3, the original error $\|f(A)v - f(A_m)v\|$ to be investigated can be reduced to a rational best approximation problem on the left complex half-plane.

Lemma 4. (Near-optimality) *For any matrix A with $W(A) \subseteq \mathbb{C}_0^-$ and any function f analytic in $\mathbb{C}_0^-$, the estimate*

$$\|f(A)v - f(A_m)v\| \leq 2\|v\| \min_{r \in \mathcal{R}_{m-1}} \sup_{z \in \mathbb{C}_0^-} |f(z) - r(z)| \,,$$

holds true, where $\mathcal{R}_{m-1} = \mathcal{P}_{m-1}/(\gamma - \cdot)^{m-1}$.

Proof. Due to Lemma 3, we have $r(A)v = r(A_m)v$ for every rational function $r \in \mathcal{R}_{m-1}$ and therefore

$$\|f(A)v - f(A_m)v\| \leq \|f(A) - r(A)\|\|v\| + \|f(A_m) - r(A_m)\|\|v\| \,. \qquad (4)$$

For matrices A with $W(A) \subseteq \mathbb{C}_0^-$ and a function g that is analytic in $\mathbb{C}_0^-$, von Neumann has shown in [24] that

$$\|g(A)\| \leq \sup_{z \in \mathbb{C}_0^-} |g(z)| \,. \qquad (5)$$

As an orthogonal projector, P_m is self-adjoint and we conclude for every vector $x \in \mathbb{C}^N$ that

$$\mathrm{Re}(A_m x, x) = \mathrm{Re}(P_m A P_m x, x) = \mathrm{Re}(A P_m x, P_m x) = \mathrm{Re}(Ay, y) \leq 0$$

by our assumption $W(A) \subseteq \mathbb{C}_0^-$. Hence, von Neumann's result can be applied to both terms in (4). Taking then the minimum over all $r \in \mathcal{R}_{m-1}$, the theorem is proved. □

After some minor modifications, all presented results in this section remain valid for the standard Krylov subspace method as well as general rational Krylov methods. For functions f that are analytic in a neighborhood of $W(A)$, the findings transfer to matrices with an arbitrary field-of values by using Crouzeix's inequality (see [5])

$$\|f(A)\| \leq C \sup_{z \in W(A)} |f(z)| \,, \quad C \leq 11.08 \,.$$

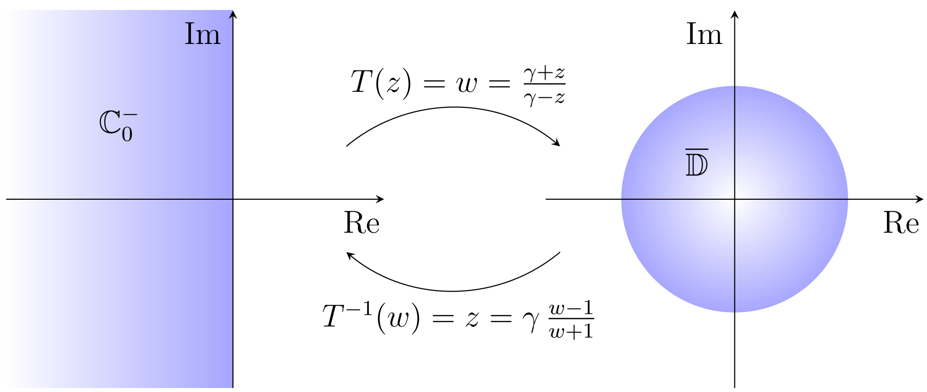

Figure 2: Transformation of $\mathbb{C}_0^-$ onto $\overline{\mathbb{D}}\backslash\{-1\}$ and vice versa.

3. Transformation to the unit disk

Let the function f be analytic in $\mathbb{C}_0^-$ and let $A \in \mathbb{C}^{N\times N}$ be a stiff matrix with $W(A) \subseteq \mathbb{C}_0^-$. The first step to obtain an error bound for the approximation of $f(A)v$ in the shift-and-invert Krylov subspace is to transform the corresponding scalar approximation problem to an approximation problem on the unit disk. Subsequently, trigonometric approximation results can be applied to the transformed problem.

According to Lemma 4, we are concerned with the problem of approximating the scalar function $f(z)$ uniformly on $\mathbb{C}_0^-$ by a rational function $r(z)$ with $r \in \mathcal{R}_{m-1}$. With respect to Lemma 1, we can investigate the best approximation problem

$$\min_{c_k} \left| f(z) - \sum_{k=0}^{m-1} c_k \left(\frac{\gamma+z}{\gamma-z}\right)^k \right| \quad \text{instead of} \quad \min_{a_k} \left| f(z) - \sum_{k=0}^{m-1} a_k \,\frac{1}{(\gamma-z)^{m-1}} \right| .$$

We now make use of the Möbius transformation T and its inverse T^{-1} given by

$$T(z) := w = \frac{\gamma+z}{\gamma-z} \qquad \Longleftrightarrow \qquad z = T^{-1}(w) = \gamma\,\frac{w-1}{w+1}$$

to map the left complex half-plane $\mathbb{C}_0^-$ onto the closed unit disk $\overline{\mathbb{D}}\backslash\{-1\}$ and vice versa, cf. Figure 2. If we define the set

$$\begin{aligned}\mathcal{M} := \{f : \mathbb{C} \to \mathbb{C} \,:\, & f \text{ analytic in } \mathbb{C}_0^- \text{ and} \\ & \exists\, c \in \mathbb{C} \text{ with } f(z) \xrightarrow{|z|\to\infty} c \;\forall\, z \in \mathbb{C}_0^- \}\,,\end{aligned} \tag{6}$$

the transformed function $\widetilde{f}(w) := f\big(T^{-1}(w)\big)$ is for every function $f \in \mathcal{M}$ analytic in $\overline{\mathbb{D}}\backslash\{-1\}$ and can be continuously extended to -1 by setting $\widetilde{f}(-1) = c$. With the Möbius transformation T and (5), it follows for every $r \in \mathcal{R}_{m-1}$ that

$$\begin{aligned}
\|f(A) - r(A)\| &\leq \sup_{z\in\mathbb{C}_0^-}\left|f(z) - \sum_{k=0}^{m-1} c_k \left(\frac{\gamma+z}{\gamma-z}\right)^k\right| \\
&\leq \max_{w\in\overline{\mathbb{D}}}\left|f\left(\gamma\,\frac{w-1}{w+1}\right) - \sum_{k=0}^{m-1} c_k w^k\right| \\
&\leq \max_{w\in\overline{\mathbb{D}}}\left|\widetilde{f}(w) - \sum_{k=0}^{m-1} c_k w^k\right| = \max_{t\in[0,2\pi)}\left|\widehat{f}(t) - \sum_{k=0}^{m-1} c_k e^{itk}\right| \qquad (7)
\end{aligned}$$

with the 2π-periodic function $\widehat{f}(t) := f\big(T^{-1}(e^{it})\big)$. The last equality is due to the maximum modulus principle. In order to find an error bound for the trigonometric approximation problem (7), we use a result by Achyèser in [1] for 2π-periodic real-valued functions. It is based on the well-known Jackson inequality and involves the following modulus of smoothness.

Definition 5. *For a continuous 2π-periodic function g and $\delta > 0$, we define the modulus of continuity*

$$\omega(g,\delta) = \sup_{0<h\leq\delta}\max_{t\in[0,2\pi)} |g(t+h) - g(t)|\,.$$

Generic constants are hereinafter denoted by $C(prm_1, prm_2, \ldots)$, where C depends only on the parameters in brackets.

Theorem 6. (Achyèser [1]) *Let g be a real-valued and 2π-periodic function which is n times continuously differentiable and let*

$$a_k = \frac{1}{\pi}\int_0^{2\pi} g(t)\cos(kt)\,dt\,, \quad b_k = \frac{1}{\pi}\int_0^{2\pi} g(t)\sin(kt)\,dt$$

for $k = 1,\ldots,m-1$ be the Fourier coefficients of the function g. Then there exists a trigonometric polynomial of degree $m-1$

$$J_{m,n}(g,t) = \frac{a_0}{2} + \sum_{k=1}^{m-1} D_k(m,n)\big(a_k\cos(kt) + b_k\sin(kt)\big) \qquad (8)$$

with coefficients $D_k(m,n) \in \mathbb{R}$, that are defined as in [1] and that depend on m and n, such that

$$\max_{t\in[0,2\pi)} |g(t) - J_{m,n}(g,t)| \leq \frac{C(n)}{m^n}\, \omega\big(g^{(n)}, \tfrac{1}{m}\big)\,,$$

where the constant $C(n)$ depends only on n.

Since Theorem 6 can be used only for real-valued functions, we have to split $\widehat{f}$ into its real and imaginary part, in order to subdivide our problem into two real approximation problems. Moreover, it must be taken into account that the trigonometric approximation of $\mathrm{Re}[\widehat{f}(t)]$ and $\mathrm{Im}[\widehat{f}(t)]$ is coupled by the common coefficients c_k in (7). The next lemma shows that the special form of the Fourier coefficients allows us to approximate the real and imaginary part of $\widehat{f}(t)$ independently of each other.

Lemma 7. *Let $\widetilde{f}$ be analytic in $\mathbb{D}$ and continuous on $\overline{\mathbb{D}}$. We denote the Fourier coefficients of the real part $\mathrm{Re}[\widetilde{f}(e^{it})] = \mathrm{Re}[\widehat{f}(t)]$ and the imaginary part $\mathrm{Im}[\widetilde{f}(e^{it})] = \mathrm{Im}[\widehat{f}(t)]$ by a_k^{Re}, b_k^{Re}, a_k^{Im}, and b_k^{Im}. These coefficients satisfy*

$$a_k^{\mathrm{Re}} = b_k^{\mathrm{Im}} \quad \textit{and} \quad b_k^{\mathrm{Re}} = -a_k^{\mathrm{Im}} \quad \textit{for} \quad k \geq 1\,.$$

Proof. For $k \geq 1$, the function $\widetilde{f}(w)w^{k-1}$ is analytic in $\mathbb{D}$ and continuous on $\overline{\mathbb{D}}$. Using Cauchy's integral theorem, we obtain

$$\begin{aligned} 0 &= \int_{\partial\mathbb{D}} \widetilde{f}(w)w^{k-1}\,dw = \int_0^{2\pi} \widetilde{f}(e^{it})ie^{ikt}\,dt \\ &= \int_0^{2\pi} \big(\mathrm{Re}[\widehat{f}(t)] + i\,\mathrm{Im}[\widehat{f}(t)]\big)\big(i\cos(kt) - \sin(kt)\big)\,dt \\ &= -\pi\,(b_k^{\mathrm{Re}} + a_k^{\mathrm{Im}}) + i\,\pi\,(a_k^{\mathrm{Re}} - b_k^{\mathrm{Im}})\,, \end{aligned}$$

which proves the assertion. □

Now, Lemma 7 enables us to estimate the error of the approximation of $\widehat{f}$ by a complex trigonometric polynomial with the help of Theorem 6.

Lemma 8. *Let $f \in \mathcal{M}$ and let $\widehat{f} = f\big(T^{-1}(e^{i\,\cdot})\big)$ be n times continuously differentiable. Then the best trigonometric approximation of degree $m-1$ for $\widehat{f}$ can be bounded by*

$$\min_{c_k} \max_{t\in[0,2\pi)} \left| \widehat{f}(t) - \sum_{k=0}^{m-1} c_k e^{itk} \right| \le \frac{C(n)}{m^n}\, \omega\big(\widehat{f}^{(n)}, \tfrac{1}{m}\big)$$

with a constant $C(n)$ that depends only on n.

Proof. With regard to Theorem 6 and Lemma 7, the idea to bound the best trigonometric approximation error for $\widehat{f}$ is to choose special coefficients

$$c_0^* = a_0^* - ib_0^*\,, \quad c_k^* = D_k(m,n)(a_k^* - ib_k^*)\,,$$

where the constants $D_k(m,n)$ are defined as in (8). The coefficients

$$a_k^* := a_k^{\mathrm{Re}} = b_k^{\mathrm{Im}}\,, \quad b_k^* := b_k^{\mathrm{Re}} = -a_k^{\mathrm{Im}}\,, \quad k = 1, \dots, m-1$$

are the Fourier coefficients of $\mathrm{Re}[\widehat{f}(t)]$ and $\mathrm{Im}[\widehat{f}(t)]$, respectively. Moreover, we set $a_0 = a_0^{\mathrm{Re}}/2$ and $b_0 = -a_0^{\mathrm{Im}}/2$. With this particular choice for the coefficients of the trigonometric polynomial, we obtain by Theorem 6 that

$$\begin{aligned}
\inf_{c_k} \max_{t\in[0,2\pi)} \left| \widehat{f}(t) - \sum_{k=0}^{m-1} c_k e^{itk} \right| &\le \max_{t\in[0,2\pi)} \left| \widehat{f}(t) - \sum_{k=0}^{m-1} c_k^* e^{itk} \right| \\
&\le \max_{t\in[0,2\pi)} \left| \mathrm{Re}[\widehat{f}(t)] - \frac{a_0^{\mathrm{Re}}}{2} - \sum_{k=1}^{m-1} D_k(m,n)\big(a_k^{\mathrm{Re}}\cos(kt) + b_k^{\mathrm{Re}}\sin(kt)\big) \right| \\
&+ \max_{t\in[0,2\pi)} \left| \mathrm{Im}[\widehat{f}(t)] - \frac{a_0^{\mathrm{Im}}}{2} - \sum_{k=1}^{m-1} D_k(m,n)\big(a_k^{\mathrm{Im}}\cos(kt) + b_k^{\mathrm{Im}}\sin(kt)\big) \right| \\
&\le \frac{C(n)}{m^n}\left[\omega\big(\mathrm{Re}[\widehat{f}]^{(n)}, \tfrac{1}{m}\big) + \omega\big(\mathrm{Im}[\widehat{f}]^{(n)}, \tfrac{1}{m}\big)\right].
\end{aligned}$$

Furthermore, we have

$$\left| \mathrm{Re}[\widehat{f}(t+h)]^{(n)} - \mathrm{Re}[\widehat{f}(t)]^{(n)} \right| \le \left| \widehat{f}^{(n)}(t+h) - \widehat{f}^{(n)}(t) \right|$$

and thus

$$\omega\big(\mathrm{Re}[\,\widehat{f}\,]^{(n)}, \tfrac{1}{m}\big) = \sup_{0<h\leq\frac{1}{m}} \max_{t\in[0,2\pi)} \Big|\mathrm{Re}[\widehat{f}(t+h)]^{(n)} - \mathrm{Re}[\widehat{f}(t)]^{(n)}\Big|$$

$$\leq \sup_{0<h\leq\frac{1}{m}} \max_{t\in[0,2\pi)} \Big|\widehat{f}^{(n)}(t+h) - \widehat{f}^{(n)}(t)\Big| = \omega\big(\widehat{f}^{(n)}, \tfrac{1}{m}\big).$$

The same holds true, if we replace the real part by the imaginary part everywhere. Altogether, the assertion of our lemma follows. □

Summarizing the findings above, we now obtain an estimate for the convergence rate of the shift-and-invert Krylov subspace approximation that depends only on the smoothness properties of the transformed function $\widehat{f}$ on the boundary of the unit disk.

Theorem 9. *Let $f \in \mathcal{M}$ and $W(A) \subseteq \mathbb{C}_0^-$. Provided that $\widehat{f} = f\big(T^{-1}(e^{i\,\cdot})\big)$ is n-times continuously differentiable, the error of the shift-and-invert Krylov approximation for $f(A)v$ is bounded by*

$$\|f(A)v - f(A_m)v\| \leq \frac{C(n)}{m^n}\,\omega\big(\widehat{f}^{(n)}, \tfrac{1}{m}\big)\|v\|\,, \tag{9}$$

where $A_m = P_m A P_m$ and P_m is the orthogonal projection onto $\mathcal{Q}_m(A,v)$.

Proof. The statement follows immediately with the help of Lemma 4, relation (7), and Lemma 8. □

Since the error bound (9) does not depend on $\|A\|$, we have a uniform convergence for all matrices with an arbitrary field-of-values in the left complex half-plane. With regard to stiff matrices A stemming from a spatial discretization of some differential operator, the convergence is therefore grid-independent.

4. Error bounds for the φ-functions

In the context of exponential integrators, we would now like to know what is to be expected for the case $f = \varphi_\ell$. It is easy to check that the φ-functions belong to $\mathcal{M}$ with $c = 0$ in (6). Consequently, Theorem 9 can be used to bound the error for the approximation of $\varphi_\ell(A)v$ in the shift-and-invert Krylov subspace $\mathcal{Q}_m(A,v)$. Following the considerations above, we have to analyze $\widehat{\varphi}_\ell = \varphi_\ell\big(T^{-1}(e^{i\,\cdot})\big)$ with respect to its smoothness properties. In doing so, it is easier to estimate separately the moduli of continuity for the n-th derivative of the real and imaginary part instead of investigating directly $\widehat{\varphi}_\ell^{(n)}$. The subsequent lemma will prove useful for this purpose.

Lemma 10. *For $x \in \mathbb{R}$, the functions $x\sin\left(\frac{1}{x}\right)$ and $x\cos\left(\frac{1}{x}\right)$ are $\frac{1}{2}$ - Hölder continuous on any bounded interval.*

Proof. Using $2xy = x^2 + y^2 - (y-x)^2$, we find

$$\begin{aligned}
&\Big|y\sin\left(\tfrac{1}{y}\right) - x\sin\left(\tfrac{1}{x}\right)\Big|^2 = \Big|y^2\sin^2\left(\tfrac{1}{y}\right) - 2xy\sin\left(\tfrac{1}{y}\right)\sin\left(\tfrac{1}{x}\right) + x^2\sin^2\left(\tfrac{1}{x}\right)\Big| \\
&= \Big|\big[\sin\left(\tfrac{1}{y}\right) - \sin\left(\tfrac{1}{x}\right)\big]\big[y^2\sin\left(\tfrac{1}{y}\right) - x^2\sin\left(\tfrac{1}{x}\right)\big] + (y-x)^2\sin\left(\tfrac{1}{x}\right)\sin\left(\tfrac{1}{y}\right)\Big| \\
&\le 2\Big|y^2\sin\left(\tfrac{1}{y}\right) - x^2\sin\left(\tfrac{1}{x}\right)\Big| + |y-x|^2\,.
\end{aligned}$$

Since $x^2\sin\left(\frac{1}{x}\right)$ is Lipschitz continuous on every bounded interval, we conclude by taking the square root that

$$\Big|y\sin\left(\tfrac{1}{y}\right) - x\sin\left(\tfrac{1}{x}\right)\Big| \le C|y-x|^{\frac{1}{2}}\,.$$

For the second function $x\cos\left(\frac{1}{x}\right)$, the claim follows analogously. □

With these preliminaries, we are now prepared to establish an error bound for the shift-and-invert Krylov approximation of $\varphi_\ell(A)v$.

Theorem 11. *Let A be a matrix with $W(A) \subseteq \mathbb{C}_0^-$ and let $A_m = P_mAP_m$, where P_m denotes the orthogonal projection onto $\mathcal{Q}_m(A,v)$. Then we have*

$$\|\varphi_\ell(A)v - \varphi_\ell(A_m)v\| \le \frac{C(\ell,\gamma)}{m^{\frac{\ell}{2}}}\,\|v\|\,, \quad \ell \ge 1\,.$$

Proof. Our investigations are limited to the study of $\omega\big(\mathrm{Re}[\widehat{\varphi}_\ell]^{(n)}, \frac{1}{m}\big)$. The modulus of continuity for the imaginary part can be estimated in a similar way. We start with the observation that

$$\frac{e^{it}-1}{e^{it}+1} = i\tan\left(\tfrac{t}{2}\right)\,. \tag{10}$$

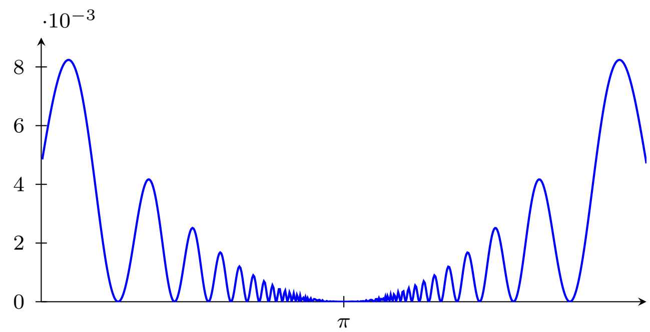

Figure 3: Plot of $\mathrm{Re}[\widehat{\varphi}_\ell(t)]$ for $t \in [3, 3.28]$, $\ell = 2$, and $\gamma = 1$.

Since $\mathrm{Re}[\widehat{\varphi}_\ell(t)] = \mathrm{Re}[\varphi_\ell\big(i\gamma \tan(\frac{t}{2})\big)]$ is infinitely often differentiable on $\mathbb{R}\backslash\{k\pi\}$, $k \in \mathbb{Z}$, we analyze the smoothness properties on the interval $(k\pi - \delta, k\pi + \delta)$ for $0 < \delta < \pi$ and $k \in \mathbb{Z}$. Due to the 2π-periodicity, it suffices to consider the behavior of $\mathrm{Re}[\widehat{\varphi}_\ell(t)]$ on $\mathbb{T}_\pi := (\pi - \delta, \pi + \delta)$, see Figure 3. In the following, we will distinguish between the two cases ℓ even and ℓ odd.

(i) ℓ even: Using (2) and (10), we obtain

$$\mathrm{Re}[\widehat{\varphi}_\ell(t)] = (-1)^{\frac{\ell}{2}} \left[\frac{\cos\big(\gamma \tan(\frac{t}{2})\big)}{\big(\gamma \tan(\frac{t}{2})\big)^\ell} - \sum_{k=0}^{\frac{\ell}{2}-1} (-1)^k \frac{\gamma^{2k-\ell}}{(2k)!} \tan^{2k-\ell}\left(\tfrac{t}{2}\right) \right].$$

The second term on the right-hand side belongs to $C^\infty(\mathbb{T}_\pi)$. A detailed analysis of the first term shows that overall $\mathrm{Re}[\widehat{\varphi}_\ell] \in C^{\frac{\ell}{2}-1}(\mathbb{T}_\pi)$. Moreover, we find by the mean value theorem on the interval $\mathbb{T}_\pi$ that

$$\omega\big(\mathrm{Re}[\widehat{\varphi}_\ell]^{(\frac{\ell}{2}-1)}, \tfrac{1}{m}\big) \le \frac{C(\ell, \gamma)}{m}.$$

(ii) ℓ odd: Because of

$$\mathrm{Re}[\widehat{\varphi}_\ell(t)] = (-1)^{\frac{\ell-1}{2}} \left[\frac{\sin\big(\gamma \tan(\frac{t}{2})\big)}{\big(\gamma \tan(\frac{t}{2})\big)^\ell} + \sum_{k=0}^{\frac{\ell-1}{2}-1} (-1)^{k+1} \frac{\gamma^{2k-\ell+1}}{(2k+1)!} \tan^{2k-\ell+1}\left(\tfrac{t}{2}\right) \right],$$

similar arguments can be used to the second case. This time, we have $\mathrm{Re}[\widehat{\varphi}_\ell] \in C^{\lfloor \frac{\ell}{2} \rfloor}(\mathbb{T}_\pi)$. The second term on the right-hand side is again infinitely often differentiable on $\mathbb{T}_\pi$. Differentiating the first expression $\lfloor \frac{\ell}{2} \rfloor$ times, we obtain a linear combination of terms of the type

$$g_1^k(t) := \frac{\sin\left(\gamma \tan(\frac{t}{2})\right)}{\left(\gamma \tan(\frac{t}{2})\right)^k} \quad \text{and} \quad g_2^k(t) := \frac{\cos\left(\gamma \tan(\frac{t}{2})\right)}{\left(\gamma \tan(\frac{t}{2})\right)^k},$$

where $k \geq 1$. Critical are the terms with $k = 1$, since they have the least smoothness. This is where Lemma 10 comes into play. Setting $x = \left(\gamma \tan(\frac{t}{2})\right)^{-1}$ and $y = \left(\gamma \tan(\frac{t+1/m}{2})\right)^{-1}$, the estimate

$$\left|g_j^1\left(t + \tfrac{1}{m}\right) - g_j^1(t)\right| \leq C \left| \frac{1}{\gamma \tan\left(\frac{t+1/m}{2}\right)} - \frac{1}{\gamma \tan\left(\frac{t}{2}\right)} \right|^{\frac{1}{2}} \leq \frac{C(\gamma)}{\sqrt{m}}$$

for $t \in \mathbb{T}_\pi$ and $j \in \{1, 2\}$ holds true, where the second inequality results from the mean value theorem. Hence, we can conclude

$$\omega\left(\mathrm{Re}[\widehat{\varphi}_\ell]^{\lfloor \frac{\ell}{2} \rfloor}, \tfrac{1}{m}\right) \leq \frac{C(\ell, \gamma)}{\sqrt{m}}.$$

Note that $m^{-\lfloor \frac{\ell}{2} \rfloor} \cdot m^{-\frac{1}{2}} = m^{-\frac{\ell}{2}}$.

The conducted analysis concludes our proof by using Theorem 9. □

With regard to the application of the shift-and-invert Krylov subspace method within exponential integrators, we are interested in the approximation of $\varphi_\ell(\tau A)v$, $\tau > 0$, instead of $\varphi_\ell(A)v$. Since $W(\tau A) \subseteq \mathbb{C}_0^-$ on the condition that $W(A) \subseteq \mathbb{C}_0^-$, Theorem 11 transfers to the matrix τA with the same constants.

Corollary 12. *Suppose that $W(A) \subseteq \mathbb{C}_0^-$ and $\tau > 0$. Let P_m be the orthogonal projection onto $\mathcal{Q}_m(\tau A, v)$ and $A_m = P_m A P_m$, then*

$$\|\varphi_\ell(\tau A)v - \varphi_\ell(\tau A_m)v\| \leq \frac{C(\ell, \gamma)}{m^{\frac{\ell}{2}}} \|v\|, \quad \ell \geq 1.$$

By now the question arises whether the shift $\gamma > 0$ can be optimally chosen. An answer to this question is given in [7]. There it is shown by a tedious calculation that for the choice

$$\gamma = m^\alpha \quad \text{with} \quad \alpha = \frac{r - \frac{\ell}{2}}{r + \frac{\ell}{2}}, \quad r > \frac{\ell}{2} + 1, \tag{11}$$

we obtain the improved error bound

$$\|\varphi_\ell(\tau A)v - \varphi_\ell(\tau A_m)v\| \leq \frac{C(\ell,\gamma,r)}{m^{\frac{\ell}{2}(1+\alpha)}} \|v\| .$$

However, this strategy to choose γ has two shortcomings: As γ depends on m, the number of iteration steps must be known in advance. Furthermore, the convergence rate is getting faster and faster by increasing the parameter r, but at the price that the constant $C(\ell,\gamma,r)$ grows with r.

Besides the φ-functions, exponential integrators involve products of the matrix exponential of τA times a vector. Since the exponential function does not belong to $\mathcal{M}$, Theorem 9 cannot be applied in this case. But this fact is not a problem due to the relation $e^{\tau A}v = v + \tau\varphi_1(\tau A)Av$. Hence, we can just approximate $\varphi_1(\tau A)$ times Av in $\mathcal{Q}_m(\tau A, Av)$ instead of approximating $e^{\tau A}v$ directly. For vectors v resulting from the discretization of some smooth initial data, it is shown in [9] that also a direct approximation of $e^{\tau A}v$ in $\mathcal{Q}_m(\tau A, v)$ is possible.

5. Numerical experiments

In this section, we illustrate our error analysis at first by a small test example. Then we proceed with a spectral and a finite-element discretization of two different wave equations in 1D and 2D.

5.1. Test example

In order to validate our findings numerically, we start with a simple test example which shows that the behavior of the approximation error corresponds to the predicted convergence rate in Theorem 11. For demonstration purposes, we take a dense and normal matrix A of dimension 2000 with eigenvalues $i, 2i, \ldots, 2000i$ on the imaginary axis and a random vector v of appropriate length.

In Figure 4, we see the obtained error curves for the approximation of $\varphi_\ell(A)v$ in the shift-and-invert Krylov subspace $\mathcal{Q}_m(A,v)$ for $\ell = 1,3,5$, and $\gamma = 1$. To compare the obtained numerical results with the error bound for the φ-functions stated above, we have inserted additional dashed lines of order $\mathcal{O}(m^{-\frac{\ell}{2}})$ into the plot.

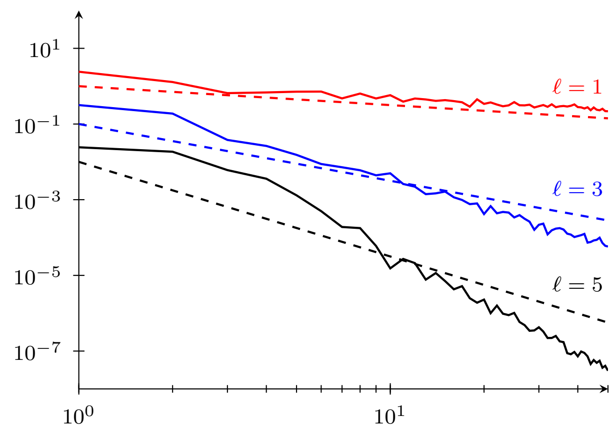

Figure 4: Error curves for the approximation of $\varphi_\ell(A)v$, $\ell = 1, 3, 5$, plotted against the dimension of $\mathcal{Q}_m(A, v)$ together with dashed lines of order $\mathcal{O}(m^{-\frac{\ell}{2}})$ corresponding to the predicted convergence rate.

5.2. 1D wave equation

On the Hilbert space $H = L^2(0,1)$, we consider the wave equation

$$\begin{aligned} &\psi'' = \Delta\psi + x && \text{for} \quad x \in (0,1)\,,\ t > 0\,,\\ &\psi(0,x) = 0\,,\ \psi'(0,x) = \frac{x^2(1-x)^2}{\|x^2(1-x)^2\|} && \text{for} \quad x \in (0,1)\,,\\ &\psi(t,0) = \psi(t,1) = 0 && \text{for} \quad t \geq 0\,. \end{aligned}$$

We discretize the problem by a spectral method and approximate the unknown solution ψ by a finite linear combination of the functions $s_k(x) = \sqrt{2}\sin(k\pi x)$, $k \in \mathbb{N}$, that form an orthonormal basis of H. These functions are eigenfunctions of the Laplacian including the homogeneous Dirichlet boundary conditions with corresponding eigenvalues $-k^2\pi^2$. If we substitute the truncated Fourier series

$$\psi(t,x) \approx \sum_{k=1}^{N} u_k(t)s_k(x)\,, \quad x \approx \sum_{k=1}^{N} f_k s_k(x)$$

into the given problem, we find

$$\sum_{k=1}^{N} u_k''(t)s_k(x) = -\sum_{k=1}^{N} k^2\pi^2 u_k(t)s_k(x) + \sum_{k=1}^{N} f_k s_k(x)\,.$$

This can be written as a system of ordinary differential equations

$$u''(t) = -Bu(t) + f\,,$$

where $B = \operatorname{diag}(\pi^2, 4\pi^2, \ldots, N^2\pi^2)$, $f = \bigl(f_k\bigr)_{k=1}^N$ contains the first N Fourier coefficients of the source term x, and $u(t) = \bigl(u_k(t)\bigr)_{k=1}^N$ is the vector with the Fourier coefficients of ψ we are looking for. If we set $v(t) = u(t)$ and $w(t) = B^{-\frac{1}{2}}u'(t)$, we obtain the first-order system

$$y'(t) = \begin{bmatrix} v(t) \\ w(t) \end{bmatrix}' = \begin{bmatrix} 0 & B^{\frac{1}{2}} \\ -B^{\frac{1}{2}} & 0 \end{bmatrix} \begin{bmatrix} v(t) \\ w(t) \end{bmatrix} + \begin{bmatrix} 0 \\ B^{-\frac{1}{2}}f \end{bmatrix} = Ay(t) + F$$

with initial values

$$y(0) = y_0 = \begin{bmatrix} v_0 \\ w_0 \end{bmatrix}, \quad v_0 = \bigl(u_k(0)\bigr)_{k=1}^N, \quad w_0 = \bigl(u_k'(0)\bigr)_{k=1}^N.$$

We take the standard Euclidian inner product for which $W(A) = [-iN\pi, iN\pi]$ such that the matrix A fits in our framework above. The solution of the transformed problem given by

$$y(\tau) = e^{\tau A}y_0 + \tau\varphi_1(\tau A)F = \tau\varphi_1(\tau A)(Ay_0 + F) + y_0$$

is now approximated in $\mathcal{Q}_m(\tau A, Ay_0 + F)$ for $\tau = 0.2$. The errors measured in the Euclidean norm are shown in Figure 5, where we used a very coarse discretization with $N = 63$ (left) and a fine one with $N = 1{,}048{,}575$ (right) basis functions. The blue dashed lines correspond to the choice $\gamma = 1$, the blue dash-dotted lines to $\gamma = m^{\frac{3}{5}}$ in accordance with (11) for $r = 2$. We clearly see that the latter choice yields a faster convergence. Moreover, we compare the results with the standard Krylov subspace approximation (red solid lines) that only works well for small N, but is impractical for finer discretizations.

5.3. 2D wave equation on a non-standard domain

In the third numerical example, we study the wave equation

$$\begin{aligned} &\psi'' = \Delta\psi - \psi && \text{for} \quad (x,y) \in \Omega\,,\ t > 0\,, \\ &\psi(0,x,y) = \psi'(0,x,y) = \psi_0(x,y) && \text{for} \quad (x,y) \in \Omega\,, \\ &\nabla_n\psi(t,x,y) = 0 && \text{for} \quad (x,y) \in \partial\Omega\,,\ t \geq 0 \end{aligned}$$

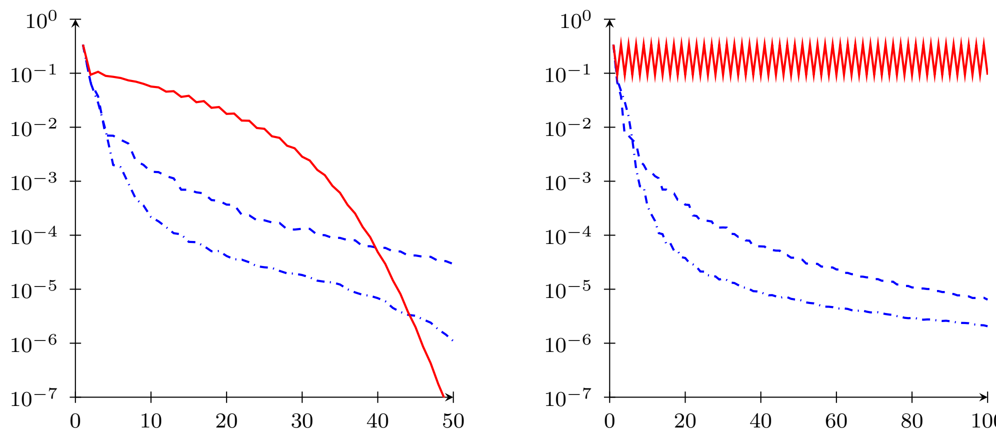

Figure 5: Error versus dimension of the Krylov subspace for the approximation of $\varphi_1(\tau A)(Ay_0 + F)$ in the standard Krylov subspace $\mathcal{K}_m(\tau A, Ay_0 + F)$ (red solid lines) and in the shift-and-invert Krylov subspace $\mathcal{Q}_m(\tau A, Ay_0 + F)$ for $\tau = 0.2$, $\gamma = 1$ (blue dashed lines) and $\gamma = m^{\frac{3}{5}}$ (blue dash-dotted lines), $N = 63$ (left) and $N = 1{,}048{,}575$ (right).

on $L^2(\Omega)$ for a non-standard domain Ω which has the shape of a unit square with a star-shaped hole in the upper left corner, see Figure 6. The discretization of the first-order formulation

$$\Psi'(t) = \begin{bmatrix} \psi(t) \\ \psi'(t) \end{bmatrix}' = \begin{bmatrix} 0 & I \\ \Delta - I & 0 \end{bmatrix} \begin{bmatrix} \psi(t) \\ \psi'(t) \end{bmatrix} = \mathcal{A}\Psi(t)$$

by linear finite elements leads to the semi-discrete problem

$$y'(t) = \begin{bmatrix} v(t) \\ w(t) \end{bmatrix}' = \begin{bmatrix} 0 & I \\ M^{-1}(S - M) & 0 \end{bmatrix} \begin{bmatrix} v(t) \\ w(t) \end{bmatrix} = Ay(t) \qquad (12)$$

with initial values $y(0) = y_0 = [v_0, u_0]^T$. For both initial values v_0 and u_0, we used a peak in the lower right corner that was evolved with the given wave equation over a time period of $\tau = 0.5$. The first component of the obtained vector y_1 is shown in Figure 6 on the right.

The matrix M in (12) is the standard mass matrix and $S - M$ represents the spatial discretization of $\Delta - I$. We now define an inner product by

$$\widetilde{z}^T Bz = (Bz, \widetilde{z}) = (z, \widetilde{z})_B \quad \text{with} \quad B = \begin{bmatrix} M - S & 0 \\ 0 & M \end{bmatrix} \qquad (13)$$

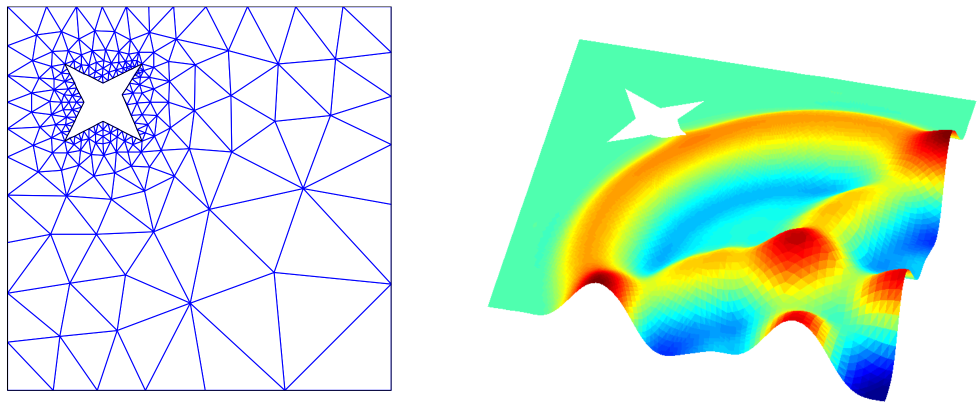

Figure 6: Domain Ω with a coarse triangulation on the left-hand side and the first component of the initial value y_1 on the right-hand side.

and denote by $\|\cdot\|_B$ its induced norm. With respect to this inner product, we have $W(A) \subseteq \mathbb{C}_0^-$, since $(Az, z)_B \in i\mathbb{R}$. For the initial value y_1 shown in Figure 6 and time step size $\tau = 0.05$, we approximate the term $\varphi_1(\tau A)Ay_1$ of the exact solution

$$y(0.5 + \tau) = e^{\tau A} y_1 = \tau\varphi_1(\tau A)Ay_1 + y_1$$

in the shift-and-invert Krylov subspace $\mathcal{Q}_m\big(\tau A, Ay_1\big)$ with shift $\gamma = 20$ and in the standard Krylov subspace $\mathcal{K}_m(\tau A, Ay_1)$. In Figure 7, the approximation error $\|\varphi_1(\tau A)Ay_1 - \varphi_1(\tau A_m)Ay_1\|_B$ is plotted against the Krylov subspace dimension m (left) and against the computing time in seconds (right) for a discretization with $189,456$ nodes and $375,808$ triangles. The occurring linear systems were solved by a multigrid method. The computation has been conducted in Matlab, Release R2015b, under Ubuntu, Release 14.04, on a quad core processor with frequency 3.5 GHz on a desktop machine.

That it is important to use a suitable inner product with regard to which the field-of-values of the matrix A lies in the left complex half-plane is demonstrated in our last numerical example. We take for both components the discrete L^2-inner product, that is $B = \operatorname{diag}(M, M)$ in (13). For this inner product, $W(A)$ protrudes into the right half-plane and does therefore no longer fulfill the requirement $W(A) \subseteq \mathbb{C}_0^-$. The resulting enormous effects on the error behavior can be seen in Figure 8 for the same parameters γ and τ as above, but a coarser discretization.

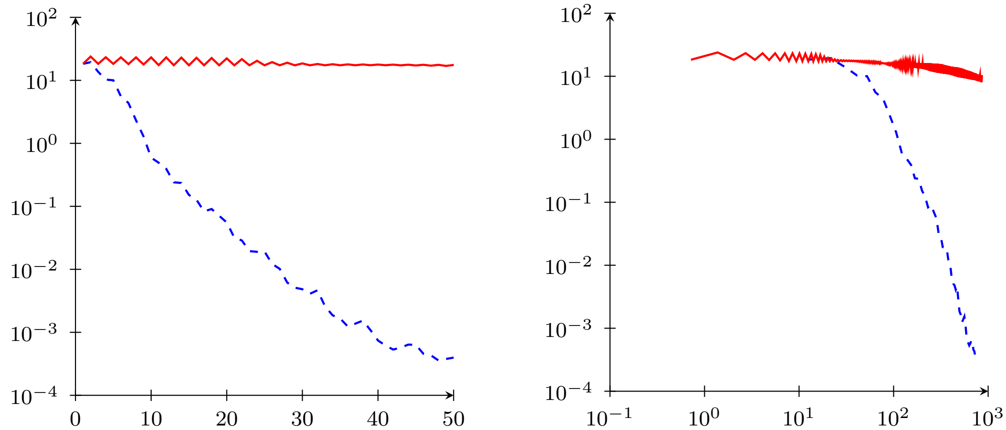

Figure 7: Error curves for the approximation of $\varphi_1(\tau A)Ay_1$ in the standard Krylov subspace $\mathcal{K}_m(\tau A, Ay_1)$ (red solid lines) and in the shift-and-invert Krylov subspace $\mathcal{Q}_m(\tau A, Ay_1)$ (blue dashed lines) plotted against the number of iteration steps (left) and the computing time in seconds (right). The parameters are chosen as $\tau = 0.05$, $\gamma = 20$, and the matrix A has dimension $378,912$.

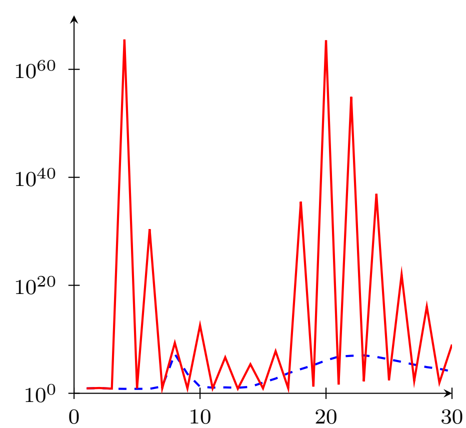

Figure 8: Error curves for the "wrong" inner product with respect to $B = \mathrm{diag}(M, M)$.

6. Conclusion

We have analyzed the convergence of the shift-and-invert Krylov subspace method for a special class of matrix functions applied to some vector, especially for the φ-functions whose efficient approximation is important within exponential integrators. For stiff matrices A with an arbitrarily large field-of-values in the left complex half-plane, $\|A\|$-independent bounds have been obtained. Therefore, we are able to approximate the φ-functions of the discretization matrix A with a convergence rate that, in contrast to the standard Krylov method, does not depend on the refinement of the spatial grid.

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