Acceleration of Contour Integration Techniques by Rational Krylov Subspace Methods

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Abstract

We suggest a rational Krylov subspace approximation for products of matrix functions and a vector appearing in exponential integrators. We consider matrices with a field-of-values in a sector lying in the left complex half-plane. The choice of the poles for our method is suggested by a fixed rational approximation based on contour integration along a hyperbola around the sector. Compared to the fixed approximation, our rational Krylov subspace method exhibits an accelerated and more stable convergence of order $\mathcal{O}(e^{-Cn})$.

Keywords: matrix functions, rational Krylov method, rational approximation, φ-functions, contour integral
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1. Introduction

In the field of exponential integrators, which form a promising class of numerical methods for the time integration of differential equations, the so-called φ-functions are of great importance. These φ-functions are given by

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

and by $\varphi_0(z) := e^z$ in the case $\ell = 0$. Another possible representation is

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

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By setting $\varphi_\ell(0) = 1/\ell!$, the φ-functions can be extended to holomorphic functions on the whole complex plane.

For the application of exponential integrators, the efficient and reliable approximation of the matrix φ-functions times a vector is an essential ingredient. In order to illustrate this, we consider the system of ordinary differential equations

$$y'(t) = Ay(t), \quad y(0) = v \quad \text{with} \quad A \in \mathbb{C}^{N\times N}, \quad v \in \mathbb{C}^N. \tag{2}$$

The solution of this problem is given as

$$y(\tau) = e^{\tau A}v = \varphi_0(\tau A)v\,,$$

which represents the simplest exponential integrator. Alternatively, the exact solution can be written as an expansion of the form

$$y(\tau) = v + \tau Av + \cdots + \frac{\tau^{\ell-1}}{(\ell-1)!}\,A^{\ell-1}v + \tau^\ell\varphi_\ell(\tau A)A^\ell v\,.$$

A fast and effective computation of the action of the matrix exponential $e^{\tau A}$ on the vector v or of the matrix function $\tau^\ell\varphi_\ell(\tau A)$ on $A^\ell v$ would thus directly lead to an efficient solution of the system (2) of ordinary differential equations.

A more involved example, where linear combinations of $\tau^\ell\varphi_\ell(\tau A)v_j$ for different vectors v_j appear, is given in [33]. Approximating the nonlinearity $N(y(t))$ in the initial value problem

$$y'(t) = Ay(t) + N(y(t))\,, \quad y(t_0) = y_0$$

by a Taylor polynomial of order s, we obtain the modified problem

$$y'(t) = Ay(t) + \sum_{j=0}^{s}\frac{t^j}{j!}\,v_j$$

with solution

$$y(t_0+\tau) = e^{\tau A}y_0 + \sum_{j=0}^{s}\sum_{\ell=0}^{j}\frac{t_0^{j-\ell}}{(j-\ell)!}\,\tau^{\ell+1}\varphi_{\ell+1}(\tau A)v_j\,.$$

Similar ideas can, for example, also be found in [21], where a kth order multistep method is obtained by approximating the nonlinearity with a suitable interpolation polynomial.

Linear combinations of the φ_ℓ-functions at possibly different time steps appear in exponential Runge–Kutta methods, for example the method given by the tableau

$$\begin{array}{c|cc} 0 & & \\ c_2 & c_2\varphi_1(c_2\tau A) & \\ \hline & \varphi_1(\tau A) - \frac{1}{c_2}\varphi_2(\tau A) & \frac{1}{c_2}\varphi_2(\tau A) \end{array} \tag{3}$$

This method has been proposed by Strehmel and Weiner in [36] and requires the evaluation of φ_1 at time τ and $c_2\tau$, and of φ_2 at time τ. The method is also discussed as a part of Example 2.18 in the review [19] on exponential integrators by Hochbruck and Ostermann.

Since exponential integrators may need evaluations of the matrix φ-functions for different time step sizes τ with the same vector v, cf. (3), we study the uniform approximation of $\tau^\ell\varphi_\ell(\tau A)v$ for $\ell \geq 0$ in a time interval $[\tau_0, \tau_1]$. Thereby, we restrict our investigations to sectorial matrices A whose field-of-values lies in a sector in the left complex half-plane. Such matrices typically arise from a spatial discretization of some parabolic partial differential equation.

For the approximation of the matrix φ-functions in a special rational Krylov subspace, we derive bounds that are completely independent of the exact location and the size of the field-of-values in the sector. Therefore, the derived error bounds hold true uniformly for arbitrary space discretizations of a given parabolic differential operator, as long as the discretization matrix keeps its field-of-values in this sector that also contains the field-of-values of the corresponding operator. Any reasonable discretization of a parabolic operator is usually of that kind. An approximation of the matrix φ-functions converging independently of the refinement of the grid in space, i.e. independently of the norm of the discretization matrix A, is crucial for the efficient application within exponential integrators. The reason is that this class of integrators has the advantage that neither the temporal convergence nor the maximum possible time step size are affected by a large norm of the discretization matrix A and this beneficial property can only be preserved by an $\|A\|$-independent approximation of the occurring matrix functions.

Our idea is based on combining a contour integration method that leads to fixed rational approximations with a rational Krylov subspace method in order to speed up the convergence. When approximating the product of a matrix function $f(A)$ with some vector v, Krylov methods can take advantage of spectral properties of v in the eigenvectors of A. For example, if there is a polynomial p of small degree m such that $p(A)v = 0$, then the Krylov method for approximating $f(A)v$ stops after m iteration steps with the exact solution. In contrast, a fixed rational (or polynomial) approximation ignores such spectral effects. Furthermore, polynomial and rational Krylov methods are known to produce an approximant, that is, up to a factor of two, related to the typically unknown best polynomial or rational approximation on the field-of-values of the considered matrix (cf. [2], Proposition 3.1 and Theorem 5.2). That means, the Krylov approximant is a quasi-best approximation and this feature can accelerate the convergence significantly compared to fixed rational approximants. Using a rational Krylov method, the vector $f(A)v$ is approximated in a rational Krylov subspace that is in general of the form

$$\begin{aligned} \mathcal{Q}_m(A,v) &= \left\{ \frac{p_{m-1}(A)}{q_{m-1}(A)}\, v,\ p_{m-1} \in \mathcal{P}_{m-1} \right\} \\ &= \operatorname{span}\{v, (z_1 - A)^{-1}v, \ldots, (z_{m-1} - A)^{-1}v\}\,, \end{aligned}$$

where $\mathcal{P}_{m-1}$ denotes the space of all polynomials of degree at most $m-1$ and $q_{m-1} \in \mathcal{P}_{m-1}$ is a fixed chosen polynomial. Every different choice of the denominator q_{m-1} results in a different rational Krylov subspace method. The roots $z_1, \ldots, z_{m-1}$ of q_{m-1} are called poles of the rational Krylov subspace. In our case, we choose simple poles z_j according to the contour integration approach in [24]. The approximation of $f(A)v$ for matrices or operators A by rational Krylov subspace methods has already been investigated in a number of papers (e.g. [1, 2, 4–6, 8–11, 13–17, 20, 22, 25–30, 32, 38]). In the context of differential operators or fine space discretizations of differential operators, it has recently emerged that rational Krylov subspace methods work tremendously better than standard Krylov subspace methods based on the subspace

$$\begin{aligned} \mathcal{K}_m(A,v) &= \{p_{m-1}(A)v,\ p_{m-1} \in \mathcal{P}_{m-1}\} \\ &= \operatorname{span}\{v, Av, \ldots, A^{m-1}v\}\,. \end{aligned}$$

The paper is organized as follows. After this introduction, we briefly review the main results in [23, 24] about the numerical inversion of the Laplace transform by a quadrature rule in Section 2. In Section 3, we introduce the rational Krylov subspace based on the fixed rational approximation reviewed in Section 2 and prove our main theorem. Before a brief conclusion, several numerical experiments are reported in Section 4.

2. A contour integral approximation for the φ-functions

For the evaluation and approximation of matrix functions, suitable contour integrals combined with the trapezoidal rule have been already considered, e.g. in [18, 31, 32, 37].

In this section, we use the results by López-Fernández, Palencia, and Schädle in [23, 24] about the application of the trapezoidal rule for the inversion of sectorial Laplace transforms in order to approximate the φ-functions. The ideas in [23, 24] are based on the papers [34, 35] by Stenger about approximation methods using Whittaker's cardinal function. The classical estimate by Stenger of order $\mathcal{O}(e^{-c\sqrt{n}})$ was first improved to $\mathcal{O}(e^{-cn/\ln(n)})$ in [23] and later refined to $\mathcal{O}(e^{-cn})$ in [24]. This refinement was achieved by selecting appropriately the free occurring parameters such as, for instance, the quadrature node spacing h. Similar ideas can be found in [39], where parabolic and hyperbolic contours for the computation of the Bromwich integral are discussed.

Let $(\cdot\,,\cdot)$ be some inner product on the vector space $\mathbb{C}^N$ with associated norm $\|\cdot\|$. The induced matrix norm is also denoted by $\|\cdot\|$. In the following, we always consider matrices $A \in \mathbb{C}^{N\times N}$ with a field-of-values

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

located in a sector

$$S_\alpha = \{z \in \mathbb{C} \,|\, |\arg(-z)| \leq \alpha\}\,, \quad 0 < \alpha < \frac{\pi}{2}$$

in the left complex half-plane. Usually, such matrices stem from a spatial discretization of a parabolic operator $\mathcal{A}$ such as $\mathcal{A}\phi = \operatorname{div}(a(x)\nabla\phi) + b(x)\cdot\nabla\phi + c(x)\phi$, where ϕ belongs to the domain of the differential operator $\mathcal{A}$. All our results can be generalized to operators $\mathcal{A}$ on Hilbert spaces and some results extend to operators $\mathcal{A}$ on Banach spaces.

We want to study matrices of an arbitrary dimension and with an arbitrarily large field-of-values $W(A) \subseteq S_\alpha$ simultaneously. For this purpose, it is helpful to represent the matrix φ-functions via a Cauchy integral along the left branch of a hyperbola around the sector S_α containing the field-of-values of the considered matrix A. More precisely, we choose $\beta, d > 0$ such that the condition

$$0 < \beta - d < \beta + d < \frac{\pi}{2} - \widetilde{\alpha}\,, \quad \alpha < \widetilde{\alpha} < \frac{\pi}{2} \tag{4}$$

is fulfilled and we define the parameterization of the left branch of the hyperbola by

$$T(s) = \lambda \cdot (1 - \sin(\beta + is))\,, \quad \lambda > 0\,, \quad s \in (-\infty, \infty)\,. \tag{5}$$

The mapping T transforms the horizontal strip of width $2d$ around the real axis into a region outside the sector S_α. This region is limited by the left branches of the two hyperbolas with foci at λ corresponding to the asymptotic angles $\pi/2 - (\beta + d)$ and $\pi/2 - (\beta - d)$ that are both larger than the angle α of the sector S_α; see Figure 1 on the left-hand side.

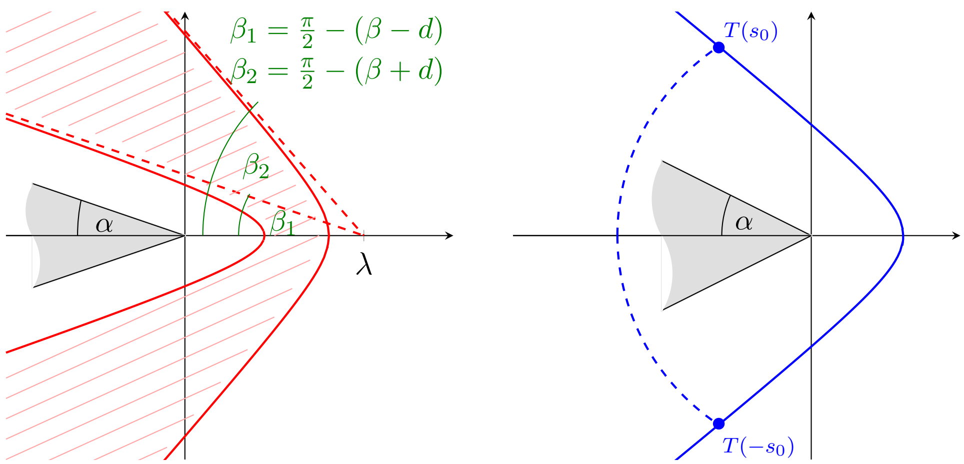

Figure 1: Shape of the horizontal strip $\{z \in \mathbb{C} \,|\, |\mathrm{Im}\, z| \leq d\}$ after the transformation by the mapping T on the left, and contour $\widetilde{\Gamma}$ in the proof of Lemma 1 on the right.

Lemma 1. *Let $A \in \mathbb{C}^{N \times N}$ be a matrix with $W(A) \subseteq S_\alpha$. Select β and d according to condition* (4)*. Then we have for $\tau \geq 0$ the representation*

$$\tau^\ell \varphi_\ell(\tau A) = \frac{1}{2\pi i} \int_\Gamma \frac{e^{\tau z}}{z^\ell} (z - A)^{-1}\, dz\,, \qquad \ell = 0, 1, 2, \ldots, \tag{6}$$

where Γ is a path with the parameterization (5)*.*

This lemma is inspired by Theorem 5.1 in [32]. The improper integral in (6) is understood in the Riemannian sense. Its existence follows from the well-known resolvent estimate (cf. [7], Section II.4)

$$\|(z-A)^{-1}\| \le \frac{M}{|z|} \quad \text{for all} \quad z \in \mathbb{C}\backslash S_{\widetilde{\alpha}}\,, \quad \alpha < \widetilde{\alpha} < \frac{\pi}{2} \tag{7}$$

which guarantees that the integral in (6) is absolutely convergent for the contour Γ running from $-i\infty$ to $+i\infty$ within the shaded area in Figure 1 on the left.

Proof (of Lemma 1). We choose a finite contour $\widetilde{\Gamma}$, that runs from $T(-s_0)$ to $T(s_0)$ on the hyperbola. Then we close the open hyperbola on the left with an arc of a circle around 0 connecting these two points in such a way that $W(A)$ is surrounded with a positive distance; cf. Figure 1 on the right. For an arbitrary $z_0 \in W(A)$, we then have

$$\tau^\ell \varphi_\ell(\tau z_0) = \frac{\tau^\ell}{2\pi i}\int_{\widetilde{\Gamma}} \frac{\varphi_\ell(\tau z)}{z-z_0}\,dz = \frac{1}{2\pi i}\int_{\widetilde{\Gamma}} \frac{e^{\tau z}}{z^\ell(z-z_0)}\,dz\,.$$

The first equality is just the Cauchy integral formula. For the second equality, we use representation (1) for the φ-functions to obtain

$$\begin{aligned}\tau^\ell \varphi_\ell(\tau z_0) &= \frac{1}{2\pi i}\int_{\widetilde{\Gamma}} \frac{e^{\tau z} - t_{\ell-1}(\tau z)}{z^\ell}\cdot\frac{1}{z-z_0}\,dz \\ &= \frac{1}{2\pi i}\int_{\widetilde{\Gamma}} \frac{e^{\tau z}}{z^\ell}\cdot\frac{1}{z-z_0}\,dz - \frac{1}{2\pi i}\int_{\widetilde{\Gamma}} \frac{1}{z-z_0}\cdot\sum_{k=0}^{\ell-1}\frac{\tau^k}{k!}\,z^{k-\ell}\,dz\,.\end{aligned}$$

With the help of the residue theorem, one can easily show that the second term vanishes. Hence, the corresponding matrix function can be written as

$$\tau^\ell \varphi_\ell(\tau A) = \frac{1}{2\pi i}\int_{\widetilde{\Gamma}} \frac{e^{\tau z}}{z^\ell}\,(z-A)^{-1}\,dz\,.$$

The proof ends by letting s_0 tend to infinity and checking that the integral over the circular arc from $T(s_0)$ to $T(-s_0)$ vanishes. □

By inserting the parameterization $T(s)$ for the contour Γ, the integral in Lemma 1 becomes

$$\tau^\ell \varphi_\ell(\tau A) = \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{e^{\tau T(s)}}{T(s)^\ell}\,T'(s)(T(s)-A)^{-1}\,ds\,.$$

We discretize this integral by the truncated trapezoidal rule with $2n + 1$ equally spaced nodes $s_k = kh$, $-n \le k \le n$ of distance h, in order to obtain the rational approximation

$$\tau^\ell \varphi_\ell(\tau A) \approx r_n(A) = \frac{h}{2\pi i} \sum_{k=-n}^{n} \frac{e^{\tau T(s_k)}}{T(s_k)^\ell} T'(s_k)(T(s_k) - A)^{-1}\,, \tag{8}$$

where $r_n \in \mathcal{P}_{2n}/q_{2n+1}$ with $q_{2n+1}(z) = \prod_{k=-n}^{n}(T(s_k) - z) \in \mathcal{P}_{2n+1}$. Now, setting $u(t) = \tau^\ell \varphi_\ell(\tau A)$ in Theorem 1 (and subsequent remarks) in [24], we have the following bound for the approximation of $\tau^\ell \varphi_\ell(\tau A)$ by the rational matrix function $r_n(A)$:

Lemma 2. *Suppose that d and β satisfy the condition* (4)*. For $\ell \ge 0$, $n \ge 1$, $\tau_0 > 0$, $\Lambda \ge 1$, $0 < \theta < 1$, and the parameter choice*

$$h = \frac{a(\theta)}{n}\,, \quad \lambda = \frac{2\pi d n(1-\theta)}{\tau_0 \Lambda a(\theta)}\,, \quad a(\theta) = \operatorname{arccosh}\left(\frac{\Lambda}{(1-\theta)\sin(\beta)}\right), \tag{9}$$

we obtain on the time interval $\tau_0 \le \tau \le \Lambda\tau_0$ the uniform estimate

$$\|\tau^\ell \varphi_\ell(\tau A) - r_n(A)\| \le C \cdot \frac{L(\lambda \tau_0 \sin(\beta - d))}{\lambda^\ell} \cdot \frac{2\epsilon_n(\theta)^\theta}{1 - \epsilon_n(\theta)} \tag{10}$$

with

$$C = M \cdot \frac{2}{\pi} \sqrt{\frac{1 + \sin(\beta + d)}{(1 - \sin(\beta + d))^{2\ell+1}}}\,, \quad \epsilon_n(\theta) = \exp\left(-\frac{2\pi d n}{a(\theta)}\right),$$

where M denotes the constant in (7)*. The function L in* (10) *is given as $L(s) = 1 + |\ln(1 - e^{-s})|$, where $L(s)$ behaves like $|\ln(s)|$ for $s \to 0+$ and tends to 1 for $s \to +\infty$.*

This convergence result for a fixed rational approximation of $\tau^\ell \varphi_\ell(\tau A)$ will now be used to construct a rational Krylov subspace method with the same poles but an improved convergence behavior.

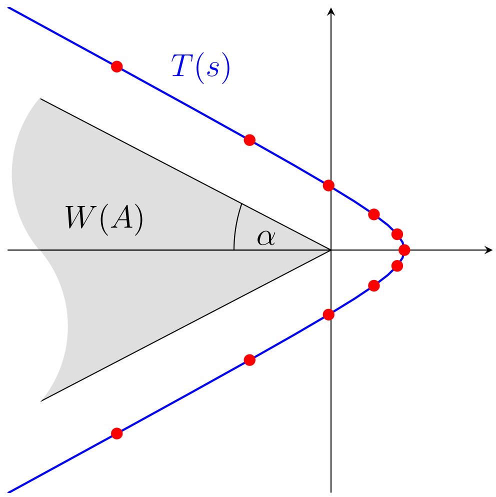

Figure 2: The field-of-values $W(A)$ of A and the location of the poles on the hyperbola T.

3. Rational Krylov subspace approximation

In this section, we consider the approximation of the vector $\tau^\ell \varphi_\ell(\tau A)v$ in the rational Krylov subspace

$$\begin{aligned}\mathcal{Q}_{2n+2}(A,v) &= \left\{ \frac{p_{2n+1}(A)}{q_{2n+1}(A)}\, v,\ p_{2n+1} \in \mathcal{P}_{2n+1} \right\} \\ &= \operatorname{span}\{v, (z_{-n}-A)^{-1}v, (z_{-(n-1)}-A)^{-1}v, \ldots, (z_n - A)^{-1}v\}\,.\end{aligned}$$

In accordance with the considerations of the previous section, we choose the poles as $z_k = T(hk)$, $k = -n, \ldots, n$, where T is the hyperbola defined in (5) winding around the field-of-values $W(A)$; see Figure 2. The fixed denominator polynomial q_{2n+1} of the rational Krylov subspace $\mathcal{Q}_{2n+2}(A,v)$ has therefore the form

$$q_{2n+1}(z) = \prod_{k=-n}^{n} \left[\lambda \cdot (1 - \sin(\beta + ikh)) - z \right], \tag{11}$$

where the parameters h, λ, and β are chosen according to (4) and (9).

The rational Krylov approximation is now defined as

$$\tau^\ell \varphi_\ell(\tau A)v \approx \tau^\ell \varphi_\ell(\tau A_n)v\,,$$

where $A_n \in \mathbb{C}^{N\times N}$ is the restriction of the matrix A to $\mathcal{Q}_{2n+2}(A,v)$ and has rank $2n+2$. This restriction is given by $A_n = P_n A P_n$, where P_n designates the orthogonal projection onto the rational Krylov subspace $\mathcal{Q}_{2n+2}(A,v)$. Let $V_n \in \mathbb{C}^{N\times(2n+2)}$ be a matrix whose columns $v_1,\dots,v_{2n+2}$ build an orthonormal basis of $\mathcal{Q}_{2n+2}(A,v)$. Then the orthogonal projector P_n is given as $V_n V_n^+$, where $V_n^+ \in \mathbb{C}^{(2n+2)\times N}$ denotes the Moore-Penrose pseudoinverse of V_n with respect to the chosen inner product on $\mathbb{C}^N$. With these notations the rational Krylov subspace approximation can be written as

$$\tau^\ell \varphi_\ell(\tau A)v \approx \tau^\ell \varphi_\ell(\tau A_n)v = \tau^\ell V_n \varphi_\ell(\tau S_n) V_n^+ v\,, \quad S_n = V_n^+ A V_n\,.$$

The function φ_ℓ then has to be evaluated only for a small square matrix S_n of dimension $2n+2 \ll N$. This can be done by standard algorithms for dense matrices.

The orthonormal basis vectors $v_1,\dots,v_{2n+2}$ can be computed by a rational Arnoldi process or Gram-Schmidt orthogonalization. In contrast to the sequential Arnoldi algorithm, the latter allows for a parallel implementation by assigning to each computing node the solution of one of the linear systems $(z_k - A)w_k = v$ for $k = -n,\dots,n$. This procedure results in a tremendous speed-up. A similar approach was carried out in [12], where matrices A with $W(A) \subseteq \{z \in \mathbb{C} \,|\, \mathrm{Re}(z) \leq 0\}$ have been considered and where the different poles of the rational Krylov subspace have been located parallel to the imaginary axis.

It is known that solving the linear systems in parallel and using a Gram-Schmidt-type orthogonalization tends to produce an ill-conditioned rational Krylov basis and numerical inaccuracies may occur during the orthogonalization. Special care needs to be taken to stabilize the algorithm. A more detailed recent discussion in the context of general rational Krylov subspace methods can be found in [3].

With the help of the results in the previous section, we are now able to state the following theorem.

Theorem 3. *Let the fixed denominator q_{2n+1} of the rational Krylov subspace $\mathcal{Q}_{2n+2}(A,v)$ be given as in* (11). *Moreover, let A be a matrix with $W(A) \subseteq S_\alpha$ and denote by A_n its restriction to $\mathcal{Q}_{2n+2}(A,v)$. We assume that the parameters are chosen according to* (4) *and* (9). *For the approximation of $\tau^\ell\varphi_\ell(\tau A)v$, $\ell \geq 0$, in $\mathcal{Q}_{2n+2}(A,v)$, we have for $\tau_0 \leq \tau \leq \Lambda\tau_0$ the uniform estimate*

$$\|\tau^\ell \varphi_\ell(\tau A)v - \tau^\ell \varphi_\ell(\tau A_n)v\| \leq \frac{C_1}{n^\ell} \cdot e^{-C_2 n} \cdot \|v\|\,, \quad n \geq 1\,, \qquad (12)$$

where the constants C_1 and C_2 depend on ℓ, d, β, and θ.

PROOF. Let $\tau \in [\tau_0, \Lambda\tau_0]$ be arbitrarily chosen. For all rational functions $r \in \mathcal{P}_{2n+1}/q_{2n+1}$ evaluated at the matrix A, the rational Krylov subspace approximation of $r(A)v$ in $\mathcal{Q}_{2n+2}(A, v)$ is exact (see [2], p. 3869). More precisely, we have

$$r(A_n)v = r(A)v \quad \text{for all} \quad r \in \mathcal{P}_{2n+1}/q_{2n+1}\,.$$

Therefore, we obtain the estimate

$$\begin{aligned}\|\tau^\ell\varphi_\ell(\tau A)v - \tau^\ell\varphi_\ell(\tau A_n)v\| &\le \|\tau^\ell\varphi_\ell(\tau A) - r(A)\|\|v\| \\ &\quad + \|\tau^\ell\varphi_\ell(\tau A_n) - r(A_n)\|\|v\|\,.\end{aligned} \tag{13}$$

The relation $A_n = P_nAP_n$ with the self-adjoint projector P_n implies for all $x \in \mathbb{C}^N$ that

$$(A_nx, x) = (AP_nx, P_nx) \subseteq S_\alpha$$

and thus $W(A_n) \subseteq S_\alpha$ by our assumption $W(A) \subseteq S_\alpha$. We now choose for r the special rational function

$$r(z) = \frac{h}{2\pi i}\sum_{k=-n}^{n}\frac{e^{\tau T(s_k)}}{T(s_k)^\ell}\,\frac{T'(s_k)}{T(s_k) - z} \in \mathcal{P}_{2n}/q_{2n+1} \subseteq \mathcal{P}_{2n+1}/q_{2n+1}$$

as in (8). Then, we use inequality (10) for both terms on the right-hand side of (13). This yields

$$\|\tau^\ell\varphi_\ell(\tau A)v - \tau^\ell\varphi_\ell(\tau A_n)v\| \le 2C\cdot\frac{L(\lambda\tau_0\sin(\beta-d))}{\lambda^\ell}\cdot\frac{2\epsilon_n(\theta)^\theta}{1-\epsilon_n(\theta)}\,\|v\|\,.$$

Thus, (12) holds true with

$$\begin{aligned}C_1 &= \frac{8M}{\pi\left(1-\exp\left(-\frac{2\pi d}{a(\theta)}\right)\right)}\cdot\sqrt{\frac{1+\sin(\beta+d)}{(1-\sin(\beta+d))^{2\ell+1}}} \\ &\quad\cdot L\left(\frac{2\pi d(1-\theta)\sin(\beta-d)}{\Lambda a(\theta)}\right)\cdot\left(\frac{\tau_0\Lambda a(\theta)}{2\pi d(1-\theta)}\right)^\ell \\ C_2 &= -\frac{2\pi d\theta}{a(\theta)}\,,\end{aligned}$$

where we used that $L(s)$ and $(1-\exp(-s))^{-1}$ are decreasing functions in $s > 0$. □

4. Numerical experiments

We start this section with a test example, where we contrast the performance of the rational Krylov subspace method with the fixed rational approximation. In a second example, we consider a convection diffusion equation whose discretization leads to a matrix with a sectorial field-of-values.

4.1. Test example

For the standard Euclidean norm, we consider the approximation of $e^A v$ in the rational Krylov subspace $\mathcal{Q}_{2n+2}(A, v)$ and compare the convergence with the fixed rational approximation in (8) that we have obtained by discretizing the above integral representation of the matrix φ-functions by a suitable quadrature rule. As test matrix, we take a normal matrix $A \in \mathbb{C}^{1000\times 1000}$ whose eigenvalues lie on the boundary of the sector $S_{\pi/4}$, so that $W(A) \subseteq S_{\pi/4}$. To be exact, the eigenvalues of A lie in the intervals $e^{\pm i(\pi-\alpha)} \cdot [1, 500]$.

The vector v is chosen as a random vector of norm one. Furthermore, we set $\beta = \pi/8$ and $d = \pi/9$ such that the assumption (4) is satisfied. The distance h of the quadrature nodes and the parameter λ of the contour T are tuned as suggested in Theorem 1 of [24] (cf. Section 2 above), where we choose $\tau_0 = 1$, $\Lambda = 1$ and $\theta = 0.5$.

According to the foregoing description, the poles of rational Krylov subspace approximation as well as those of the fixed approximation are symmetrically located along the hyperbola $T(s) = \lambda(1-\sin(\beta+is))$, $s \in (-\infty, +\infty)$, with focus λ and asymptotic angle $\pi/2 - \beta$.

In Figure 3, we plot the obtained errors of the rational Krylov subspace method (blue solid line) and the fixed rational approximation (red dashed line). We can clearly see that from the very first step the Krylov method converges significantly faster than the fixed approximation. After about the 40th iteration step, the approximation error even deteriorates for the latter method. The reason for this is that the errors which arise during the computation of the fixed rational approximation have an enormous influence on the convergence behavior for large values of n. Instead of the rational function $r_n(A)$ in (8), we have to consider in practice the expression

$$\overline{r}_n(A)v = \sum_{k=-n}^{n} \omega_k U_k v \, ,$$

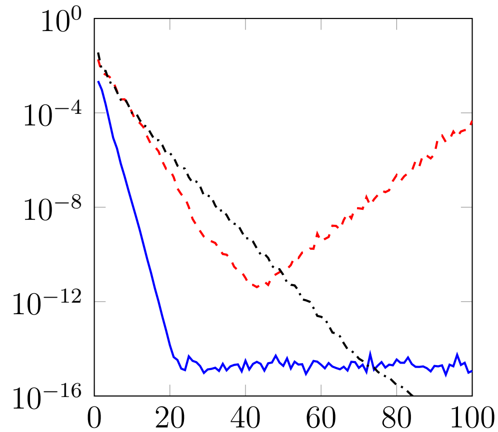

Figure 3: Comparison of the fixed (red dashed line) and the rational Krylov (blue solid line) approximation for $e^A v$ for $\theta = 0.5$. Moreover, the error of the fixed approximation is shown for the choice $\theta = 1 - 1/n$ (black dash-dotted line), in order to avoid error amplification.

where

$$U_k \approx (T(s_k) - A)^{-1} v\,, \quad \omega_k \approx \frac{h}{2\pi i}\,\frac{e^{T(s_k)} T'(s_k)}{T(s_k)^{\ell}}\,, \quad k = -n, \ldots, n\,.$$

Proceeding analogously as described in [24], a detailed analysis of the actual error $\|\varphi_\ell(A)v - \overline{r}_n(A)v\|$ reveals that an additional term of order $\mathcal{O}(\epsilon_n(\theta)^{\theta-1})$ appears which goes to infinity for $n \to \infty$. In [24], this problem of error propagation is overcome by choosing the parameter θ as $1-1/n$, which results in a slower linear convergence rate saturating at some level, but prevents error amplification. The approximation error for the fixed rational approximation using $\theta = 1 - 1/n$ is depicted in Figure 3 by the black dash-dotted line.

In contrast, this effect is not observed for the rational Krylov subspace approximation that is stable against the influence of errors; cf. Figure 3. Using a rational Arnoldi decomposition with some reorthogonalization process, it is possible to achieve nearly machine precision.

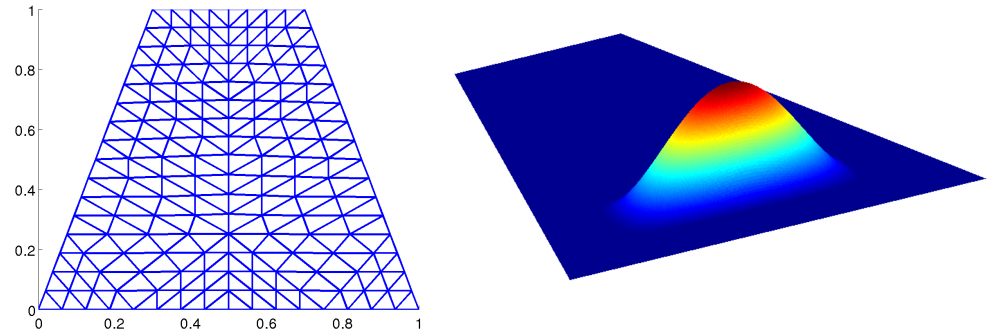

Figure 4: Domain Ω with a coarse triangulation on the left-hand side and the initial value ϕ_0 on the right-hand side.

4.2. Convection diffusion equation

On the Hilbert space $L^2(\Omega)$, we consider the convection diffusion equation

$$\begin{aligned} \phi' &= \delta\Delta\phi - b^T\nabla\phi && \text{for} \quad (x,y)\in\Omega\,,\ t>0 \\ \phi(0,x,y) &= \phi_0(x,y) && \text{for} \quad (x,y)\in\Omega \\ \phi(t,x,y) &= 0 && \text{for} \quad (x,y)\in\partial\Omega\,,\ t\geq 0\,. \end{aligned}$$

with diffusion coefficient $\delta > 0$ and velocity $b = (b_1, b_2)^T$. The domain Ω together with a coarse triangulation and the initial function ϕ_0 are shown in Figure 4. We discretize the spatial domain by finite elements, using the standard linear basis functions $\Psi_k(x,y) \in H_0^1(\Omega)$, $k = 1,\ldots,N$ on a triangular grid. This leads to the system of ordinary differential equations

$$Mu'(t) = Su(t)\,, \quad u(0) = u_0\,, \tag{14}$$

where $M, S \in \mathbb{R}^{N\times N}$ are the mass and the stiffness matrix. The coefficient vector $u(t) = (\mu_k(t))_{k=1}^N$ can be identified with the approximation

$$\phi(t,x,y) \approx \sum_{k=1}^{N} \mu_k(t)\Psi_k(x,y)$$

to the exact solution ϕ of the convection diffusion equation. The discrete problem (14) is solved by the product $e^{\tau M^{-1}S}u_0$ of the matrix exponential and the initial vector u_0. In order to determine the sector S_α that contains the field-of-values of the discretization matrix $A = M^{-1}S$, we consider the corresponding differential operator $\mathcal{A}\phi = \delta\Delta\phi - b^T\nabla\phi$. With standard techniques from functional analysis, we find that the sectorial operator $\mathcal{A}$ satisfies

$$W(\mathcal{A}) \subseteq S_\alpha\,, \quad \alpha = \arctan\left(\frac{|b_1| + |b_2|}{\delta}\right)$$

with respect to the L^2-inner product. The corresponding discrete inner product reads $(v, w)_M = w^H M v$ for $v, w \in \mathbb{C}^N$ and the mass matrix M. The field-of-values of A with respect to this M-inner product is then also contained in S_α what can be verified as follows: Since

$$(S)_{ij} = -\delta \int_\Omega \nabla\phi_i \nabla\phi_j \, d\Omega + \int_\Omega (b^T\nabla\phi_i)\phi_j \, d\Omega\,, \quad i, j = 1, \ldots, N\,,$$

we have for all $v = (\eta_k)_{k=1}^N \in \mathbb{C}^N$ the relation

$$(Av, v)_M = v^H M A v = v^H S v = (\mathcal{A}\vartheta, \vartheta)_{L^2(\Omega)} \in W(\mathcal{A}) \subseteq S_\alpha\,,$$

where $\vartheta = \sum_{k=1}^N \eta_k \Psi_k \in H_0^1(\Omega)$.

We now approximate $e^{\tau A}u_0$ in the rational Krylov subspace $\mathcal{Q}_{2n+2}(A, u_0)$. The parameters are chosen as $\tau = 0.05$, $\gamma = 10$, $\beta = 0.25$, $d = 0.2$, and $\theta = 0.5$ such that condition (4) is fulfilled. For the diffusion coefficient and the velocity, we used $\delta = 0.5$ and $b = (0, 1)^T$. To demonstrate the grid-independent convergence, we use three different refinements for the triangulation of our domain Ω leading to discretization matrices $A \in \mathbb{R}^{N\times N}$ with $N = 521$, $N = 36{,}417$, and $N = 588{,}033$. The associated approximation errors are shown in Figure 5. We see that the error curves hardly differ from each other.

For comparison, we also computed the error of the fixed approximation using the rational matrix function $r_n(A)$ in (8) which is shown in Figure 5 by the red dashed line. It becomes apparent that the difference between the rational Krylov subspace approximation and the fixed approximation is even more extreme than in the previous test example. This is a typical behavior for the rational Krylov subspace method applied to some discretized problem. The error bound (12) is only a worst case bound, often a faster convergence can be observed.

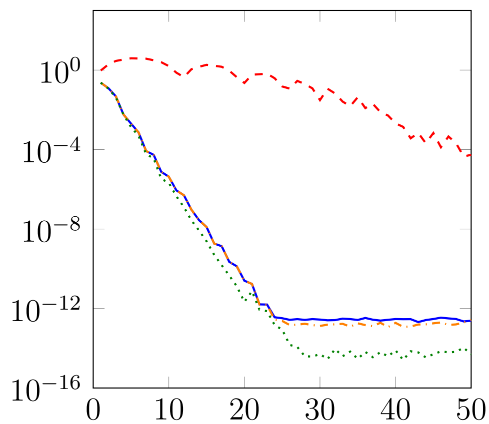

Figure 5: Error versus dimension of $\mathcal{Q}_{2n+2}(A, u_0)$ for the approximation of $e^{\tau A}u_0$. We used three different discretizations with $N = 521$ (green dotted line), $N = 36{,}417$ (orange dash-dotted line), and $N = 588{,}033$ (blue solid line) basis functions. The red dashed line shows the error of the fixed rational approximation using $r_n(A)v$ in (8).

5. Conclusion

We analyzed the approximation of $\tau^\ell \varphi_\ell(\tau A)v$ by a rational Krylov subspace method. Our study covers the case of a single time step τ as well as a time interval $\tau \in [\tau_0, \tau_1]$. The poles of the rational Krylov subspace lie on a hyperbolic contour that winds around the field-of-values of the matrix A lying inside a sectorial region in the left complex half-plane. As long as the field-of-values is contained in the sector, our error bounds are uniformly valid for matrices of arbitrary dimension and with an arbitrarily large field-of-values. In view of a matrix stemming from some spatial discretization of a differential operator, we have proven a grid-independent convergence.

The special choice of our poles in the rational Krylov subspace is based on a fixed rational approximation used in [23, 24] that is obtained by applying the trapezoidal rule to a contour integral representation of the φ-functions. Using the proposed rational Krylov method instead of the fixed approximation with the same poles, the convergence is stabilized and accelerated.

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