ANALYSIS OF PROJECTION METHODS FOR RATIONAL FUNCTION APPROXIMATION TO THE MATRIX EXPONENTIAL *

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Abstract. Krylov subspace methods for approximating the action of the matrix exponential $\exp(A)$ on a vector v are analyzed with A Hermitian and negative semidefinite. Our approach is based on approximating the exponential with the commonly employed diagonal Padé and Chebyshev rational functions, which yield a system of equations with a polynomial coefficient matrix. We derive optimality properties and error bounds for the convergence of a Galerkin-type approximation and of a computationally feasible and extensively used alternative. As complementary results, we theoretically justify the use of a popular a-posteriori error estimate, and we provide upper bounds for the components of the solution vector. Our theoretical and numerical results show that this methodology may provide an appropriate framework to devise new strategies such as more powerful acceleration schemes.

1. Introduction. The problem of numerically approximating the action of the matrix exponential $\exp(A)$ on v for a given matrix A and vector v is of great importance in a wide range of applications. In fact, it is the core of many exponential integrators for solving systems of ordinary differential equations (see [26, 25]) or time-dependent partial differential equations [17, 19]. Over the years, several methods have been proposed for approximating the exponential of a matrix; we refer to [33] for a recent survey. For A of large dimension, Krylov subspace methods for approximating $\exp(A)v$ have been successfully used for a long time; see, e.g., [36, 39], the more recent publications [19, 25, 9] and references therein. In the past few years, important contributions have appeared that have significantly increased the theoretical understanding of this approach [48, 11, 12, 24, 41]. In this paper, we restrict our attention to the case of A Hermitian and negative semidefinite, as it is often the case in real applications, although the approach can be used even for non-Hermitian A. Given an $n \times n$ matrix A, the Krylov subspace $K_m(A, v) = \text{span}\{v, Av, \dots, A^{m-1}v\}$ is characterized by the key relation

$$AV_m = V_{m+1}H_{m+1,m}, \qquad v = V_m e_1 \beta_0, \tag{1.1}$$

with $H_{m+1,m} \in \mathbb{R}^{(m+1)\times m}$ tridiagonal and $\beta_0 = \|v\|$, where $\|v\|$ is the 2-norm of v. Here and in the following, e_k denotes the kth vector of the canonical basis, whose dimension is clear from the context. In later sections, we use e_m^G and e_m^K to denote the *error* vectors for the analyzed methods. Relation (1.1), also known as the Lanczos recurrence, allows one to compute a matrix V_m whose orthonormal columns span $K_m(A, v)$, while $H_{m+1,m}$ contains the coefficients of the orthogonalization process. A common approximation in $K_m(A, v)$ is

$$\exp(A)v \approx V_m \exp(H_m) e_1 \beta_0; \tag{1.2}$$

here H_m is the (Hermitian) $m \times m$ principal part of $H_{m+1,m}$, i.e. $H_m = V_m^* A V_m$, where V_m^* is the transpose of V_m. This approximation was analyzed in [41], where it was also shown that the vector $V_m \exp(H_m) e_1 \beta_0$ represents a polynomial approximation

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to $\exp(A)v$, in which the polynomial of degree $m-1$ interpolates the exponential function in the Hermite sense on the set of eigenvalues of H_m [41, Theorem 3.3]. Our analysis aims to explore this polynomial approach but from a different perspective.

The computation of $\exp(A)$, and of $\exp(H_m)$ cannot be carried out exactly, even assuming exact arithmetic [33]; we refer to [43] for a description of current software for computing the exponential of small matrices. In practice, $\exp(H_m)$ is often very accurately approximated by means of rational functions, such as Padé or Chebyshev functions; see, e.g., [1, 20, 21, 23, 19]. Therefore, given the rational function $\mathcal{R}_{\mu,\nu}(\lambda) := \Phi_\mu(\lambda)/\Psi_\nu(\lambda)$ for some specifically chosen polynomials Ψ_μ, Φ_ν of degree μ and ν respectively, the approximate solution $V_m \exp(H_m)e_1\beta_0$ is replaced by the vector $V_m\mathcal{R}_{\mu,\nu}(H_m)e_1\beta_0$, see, e.g., the Matlab routine `expm` [32]. In the following we restrict our analysis to the case $\mu = \nu$, and thus we use $\mathcal{R}_\nu \equiv \mathcal{R}_{\nu,\nu}$; see section 3.

The aim of this paper is to increase our understanding of Krylov subspace based approximations to the exponential operator by exploiting rational functions and their approximation properties of the exponential. Rational functions may provide an appropriate framework to devise more powerful techniques, as well as to justify currently proposed approaches such as those in [6, 49]; see also section 6. In particular, we wish to set up the stage for the development of new acceleration strategies to computationally enhance the approximation process.

General results on approximation of matrix rational functions within Krylov subspaces are very limited; see for instance [51]. In practice, the theoretical as well as computational aspects associated with such approximation have not been completely addressed. We aim to contribute in filling this gap, as very general hypotheses on the rational functions are employed. Therefore, in this paper we first derive new error estimates for projection type minimization methods used to approximating the action of matrix rational functions. Our results are very general and can be applied in contexts other than the approximation of the exponential. We then derive new insightful relations for the approximation of the exponential, with the commonly employed technique in (1.2).

We start with the preliminary consideration that the approximation

$$\exp(A)v \approx \mathcal{R}_\nu(A)v = (\Psi_\nu(A))^{-1}\Phi_\nu(A)v$$

entails solving the following system of equations

$$\Psi_\nu(A)x = \Phi_\nu(A)v. \tag{1.3}$$

Note that as an alternative to solving (1.3), one could first approximately solve the system $\Psi_\nu(A)\hat{x} = v$ and then compute $x = \Phi_\nu(A)\hat{x}$. Since for $m > \nu$ it holds that $\Phi_\nu(A)v \in K_m(A, v)$, the approach (1.3) should be preferred in practice. Following [51], we analyze two procedures for solving (1.3). The first approach determines an approximation x_m by imposing a classical Galerkin condition on the residual. The second one, which we call the Krylov approximation[1], is computationally more appealing, and turns out to be equivalent to the standard procedure, namely

$$x_m = V_m\mathcal{R}_\nu(H_m)e_1\beta_0 \approx V_m \exp(H_m)e_1\beta_0. \tag{1.4}$$

For the sake of simplicity, and without loss of generality, in the following we assume that $\|v\| = 1$, so that $\beta_0 = 1$. We analyze the optimality properties of the first method,

[1]Also called Arnoldi or Lanczos approximation.

and show that the second method, although non-optimal, provides an approximate solution that is significantly close to the optimal one. By using the partial fraction expansion of $\mathcal{R}_\nu$ we derive convergence bounds for both approaches, that depend on the spectrum of A. In addition, we examine the role of the degree and the poles of both Padé and Chebyshev rational approximants in the convergence behavior as well as in the obtained error bounds.

Our convergence estimates predict linear, and not superlinear, convergence, and in this sense they are weaker than available error bounds; however, we also show that the superlinear behavior can be recovered by varying the degree ν. We stress here that our aim is not to derive better bounds than those in the literature. Instead, we wish to show that rational functions may represent a new numerical tool with no loss in convergence properties if the degree ν is taken into account.

Throughout the paper we assume exact precision arithmetic. We refer to [10] for a detailed analysis of the behavior of Krylov subspace approximations of matrix functions in finite precision computation.

This is a synopsis of the paper. In section 2 we review some basic facts on Krylov approximation of the exponential, while in section 3 we review several important properties of rational functions, that will be used extensively in the paper. In section 4 we show an optimality property associated with the Galerkin method, and provide bounds for the approximation error. In section 5 we analyze in detail the Krylov method. We first relate its approximate solution with that obtained with the optimal Galerkin approximation. Then, we derive new error estimates and compare them with those obtained for the Galerkin procedure. In section 6 we discuss some computational properties derived by using rational functions. In section 7 we analyze the Padé rational function approximation when the scaling and squaring procedure is employed to handle a matrix whose norm is significantly larger than one, while in section 8 we discuss the role of ν in the occurrence of superlinear convergence. Finally, section 9 discusses some related issues that our analysis brings to light.

2. Krylov subspace approximation to the matrix exponential. Krylov subspace approximations to the exponential have been analyzed in several papers, see, e.g., [41, 19]. However, the most significant error bounds were given in [48, 11] and later with a different approach in [24]. The authors of these papers were able to capture the so-called *superlinear* convergence of the approximation. As a reference, we recall here one of the results stated in [24] in our notation; see [48, 11] for qualitatively similar, although asymptotic bounds. We call these bounds *ideal* bounds, for reasons that will be clear in the following.

THEOREM 2.1 ([24]). *Let A be an Hermitian negative semidefinite matrix with eigenvalues in the interval $[-4\rho, 0]$. Then the error in the Lanczos approximation of $\exp(A)v$ is bounded as follows:*

$$\|\exp(A)v - V_m \exp(H_m)e_1\| \leq 10e^{-m^2/(5\rho)}, \qquad \sqrt{4\rho} \leq m \leq 2\rho,$$
$$\|\exp(A)v - V_m \exp(H_m)e_1\| \leq \frac{10}{\rho} e^{-\rho} \left(\frac{e\rho}{m}\right)^m, \qquad m \geq 2\rho.$$

Different bounds that also emphasize the superlinear character of the approximation have also been proposed in [47]; we found these latter bounds less sharp than those in [48, 11, 24], at least experimentally.

The Krylov approximation devised in (1.2) is not naturally equipped with a stopping criterion. Since the error norm $\|\exp(A)v - V_m \exp(H_m)e_1\beta_0\|$ cannot be computed explicitly as m increases, a criterion based on the quantity

$$h_{m+1,m}|e_m^* \exp(H_m)e_1\beta_0| \tag{2.1}$$

was proposed in [41, §5.2]. This criterion works well in many cases, especially when $\|A\|$ is moderate, and qualitative arguments were discussed in [41] to justify its use; a higher order estimate can also be employed, which can be easily derived from (2.1) [41]. In general, an insightful interpretation of the quantity in (2.1) in not always immediate, usually due to the lack of a definition of residual, unlike in equation based problems. An exception is the situation when the computation is related to the following initial value problem

$$\begin{cases} -Ax(t) + x'(t) = 0 \\ x(0) = v, \end{cases}$$

in which case it holds $h_{m+1,m}|e_m^* \exp(tH_m)e_1\beta_0| = \| - Ax_m(t) + x_m'(t)\|$, that is, the a-posteriori estimate is indeed the residual associated with the approximate solution $x_m(t)$; see, e.g., [7, 10]. An alternative viewpoint was proposed in [26], where the authors introduced a new concept of residual norm, by generalizing that of error norm in a functional setting. The new residual norm was shown to be equal to the estimate (2.1). With our derivation, we suggest a general role for the stopping criterion (2.1) in terms of residual associated with a matrix equation.

3. Rational function approximation. Rational functions are commonly used to accurately approximate analytic functions such as the exponential [1]. Here we review some characteristics of Chebyshev and Padé rational functions that are used in our analysis. However, several of the results in later sections apply to general rational functions and to the approximation of other smooth functions.

Let us assume that $\exp(\lambda)$ is approximated by the rational function $\mathcal{R}_\nu(\lambda)$. In this case, the quality of the approximation when using the Krylov subspace only affects part of the overall approximation. The bound

$$\begin{aligned} \|\exp(A)v - V_m \exp(H_m)e_1\| \leq \|\exp(A)v - \mathcal{R}_\nu(A)v\| + \|\mathcal{R}_\nu(A)v - V_m\mathcal{R}_\nu(H_m)e_1\| \\ + \|\mathcal{R}_\nu(H_m)e_1 - \exp(H_m)e_1\| \end{aligned}$$

emphasizes that there are two components in the error estimate: the second term on the right is the "Krylov subspace error", and it can be monitored as the chosen approximation in $K_m(A, v)$ takes place, whereas the size of the second component, corresponding to the other two terms in the bound, depends on the accuracy of the rational function approximation employed.

The first component is related to the numerical solution of the system (1.3) in the Krylov subspace. The solution of algebraic systems having a matrix function as coefficient matrix by means of Krylov subspaces has been analyzed in detail by van der Vorst in [51]; see also the recent presentation in [50]. Two distinct methods are studied in [51] for special cases of Ψ_ν and for $\Phi_\nu = 1$. In the first approach, the problem is projected onto the smaller dimension space, whereas the second approach is characterized by a sequential projection. In this paper we generalize these two methods to our framework and analyze their properties.

Several approaches have been considered for choosing the rational function approximation. In the context of one-step methods for initial value differential problems, a stable way to approximate $\exp(A)$ consists in employing diagonal Padé approximants $\mathcal{R}_\nu = \Phi_\nu/\Psi_\nu$, where Φ_ν, Ψ_ν are polynomials of degree ν; see, e.g., [26, 25] and references therein. These two polynomials satisfy $\Phi_\nu(\lambda) = \Psi_\nu(-\lambda)$, so that we can write

$$\Psi_\nu(\lambda) = \psi_\nu \cdot (\lambda - \xi_1) \cdots (\lambda - \xi_\nu), \qquad \Phi_\nu(\lambda) = \phi_\nu \cdot (\lambda + \xi_1) \cdots (\lambda + \xi_\nu). \quad (3.1)$$

Here ψ_ν and ϕ_ν are the leading term coefficients. The two polynomials are uniquely defined apart from a scaling factor. We shall assume in the following that this scaling factor is such that $\Psi_\nu(0) = \Phi_\nu(0) = 1$. The roots of Ψ_ν all have positive real part, so that those of Φ_ν have negative real part; in addition, they come in complex conjugate if their imaginary part is nonzero, and their absolute value is larger than one, and increasing with ν. The leading coefficient ψ_ν satisfies

$$|\psi_\nu| = \frac{1}{|\xi_1 \cdot \cdots \cdot \xi_\nu|} \ll 1;$$

it is positive if ν is even, and negative if ν is odd. In addition, $|\Phi_\nu(\lambda)/\Psi_\nu(\lambda)| \le 1$ for $\lambda \le 0$ [52]. Finally, for any nonpositive real λ we have $\Psi_\nu(\lambda) > 0$. In our context, this property ensures that $\Psi_\nu(A)$ is Hermitian and positive definite for any Hermitian negative semidefinite matrix A, that is $x^*\Psi_\nu(A)x > 0$ for any nonzero vector x.

In the context of parabolic partial differential equations, rational Chebyshev approximations have also been considered, see, e.g., [52, 19], which provide best rational approximations to $\exp(x)$ for $x \in (-\infty, 0]$ in the Chebyshev sense. If $\Phi_\nu(-\lambda)/\Psi_\nu(-\lambda)$ is the Chebyshev approximant for $\lambda \le 0$, then it is known that $\sup_{\lambda \le 0} |\exp(\lambda) - \Phi_\nu(-\lambda)/\Psi_\nu(-\lambda)| \approx 10^{-\nu}$; see [8, Table II]. In addition, since Ψ_ν has all strictly positive coefficients (cf. [8, Table III]), then $\Psi_\nu(x) > 0$ for $x \ge 0$, implying that $\Psi_\nu(-A)$ is positive definite for A Hermitian and negative semidefinite. The roots ξ_j of Ψ_ν appear with positive and negative real part, therefore $M_j = -A - \Re(\xi_j)I$ may be indefinite, for some ξ_j, $j = 1, \dots, \nu$. We note that the Chebyshev rational approximation uses $\Phi_\nu(-\lambda)/\Psi_\nu(-\lambda)$ with $\lambda \le 0$, whereas the Padé approximation employs $\Phi_\nu(\lambda)/\Psi_\nu(\lambda)$ with $\lambda \le 0$. In this paper we do not distinguish between the sign in the two cases, using $\Phi_\nu(\lambda)/\Psi_\nu(\lambda)$ with $\lambda \le 0$, while warning the reader that depending on the strategy used, the variable sign should be changed accordingly.

Padé approximants of degree up to $\nu = 14$ are commonly employed [23], and 10^{-14} is often considered a sufficiently good accuracy for the Chebyshev approximation. Unless otherwise specified, we thus restrict our experiments to the case $\nu \le 14$. For the sake of simplicity, we only consider equal degree approximants, whereas it is known that in the Padé approximation, $\Phi_{\nu-1}, \Psi_\nu$ also provide stable approximations in the context of stiff ordinary differential equations; see, e.g., [20]. In our analysis we use the fact that both the Padé and the Chebyshev approximants have simple poles, although the presence of multiple poles is addressed in section 7 in the context of the scaling and squaring method.

We also recall that the rational function $\mathcal{R}_\nu = \Phi_\nu/\Psi_\nu$ can be written by means of a partial fraction expansion as

$$\mathcal{R}_\nu(\lambda) = \tau_0 + \sum_{j=1}^{\nu} \frac{\tau_j}{(\lambda - \xi_j)}, \quad (3.2)$$

where $\xi_1, \dots, \xi_\nu$ are the distinct roots of Ψ_ν, $\tau_1, \dots, \tau_\nu$ are the coefficients (appearing in complex conjugates) of the expansion, and τ_0 is the remainder.

4. Convergence analysis of the Galerkin method. In this section we analyze the convergence properties of the Galerkin approximation. A Galerkin approach based on the Krylov subspace $K_m(A, v)$, approximates x in (1.3) as $x_m^G = V_m y_m^G$, by imposing that the residual $\Phi_\nu(A)v - \Psi_\nu(A)x_m^G$ be orthogonal to the Krylov subspace, namely, $V_m^*(\Phi_\nu(A)v - \Psi_\nu(A)x_m^G) = 0$. Therefore, y_m^G is computed as the solution to the system

$$V_m^* \Psi_\nu(A) V_m y = V_m^* \Phi_\nu(A) v. \tag{4.1}$$

The method is of interest from a theoretical point of view, because of its optimality properties. From a computational standpoint, the explicit computation of $V_m^* \Psi_\nu(A) V_m$ requires ν evaluations with A at each iteration, making the approach not appealing. The Krylov approximation thus represents a valuable competitive alternative, and we show that the convergence properties are indeed comparable.

We first show that the Galerkin approximate solution has a minimization property, ensuring that the error is non-increasing with m, in the considered norm; then we derive upper bounds for this error norm. All these results appear to be new.

PROPOSITION 4.1. *Let $x_\star = \mathcal{R}_\nu(A)v$ and let x_m^G be the Galerkin approximation to $x_\star$ in $K_m(A, v)$ and assume that $\Psi_\nu(A)$ is Hermitian and positive definite. Then*

$$\min_{x \in K_m(A,v)} \|x_\star - x\|_{\Psi_\nu(A)} = \|x_\star - x_m^G\|_{\Psi_\nu(A)}.$$

Proof. The result follows from imposing the Galerkin condition on the residual $\Psi_\nu(A)(x_\star - x_m)$; cf. [42, Proposition 5.2]. ∎

PROPOSITION 4.2. *Let $[\alpha, \beta]$ be the interval containing all eigenvalues of A, and assume that the hypotheses of Proposition 4.1 hold. Then*

$$\begin{aligned}\min_{x \in K_m(A,v)} \|x_\star - x\|^2_{\Psi_\nu(A)} &= \min_{q \in \mathbb{P}_{m-1}} \|x_\star - q(A)v\|^2_{\Psi_\nu(A)} \\ &\le \min_{q \in \mathbb{P}_{m-1}} \max_{\lambda \in [\alpha,\beta]} \left|1 - \mathcal{R}_\nu(\lambda)^{-1} q(\lambda)\right|^2 \|v\|^2_{\Psi_\nu(A)}.\end{aligned}$$

Proof. Let $u_1, \ldots, u_n$ be the unit norm eigenvectors of A associated with the eigenvalues $\lambda_1, \ldots, \lambda_n$. Define $\chi_i := u_i^* x_\star$ and $s(\lambda) := 1 - q(\lambda)(\mathcal{R}_\nu(\lambda))^{-1}$. We have $x_\star - q(A)v = \left(I - q(A)(\mathcal{R}_\nu(A))^{-1}\right) x_\star = \sum_{i=1}^n u_i s(\lambda_i)\chi_i$, so that

$$\begin{aligned}\|x_\star - q(A)v\|^2_{\Psi_\nu(A)} &= \langle x_\star - q(A)v, \Psi_\nu(A)(x_\star - q(A)v) \rangle \\ &= \sum_{i=1}^n \Psi_\nu(\lambda_i)(s(\lambda_i))^2 \chi_i^2 \le \max_{\lambda \in [\alpha,\beta]} |s(\lambda)|^2 \|v\|^2_{\Psi_\nu(A)}. \qquad \square\end{aligned}$$

We next provide a bound for the polynomial min-max problem in Proposition 4.2. In the sequel we use the following definitions. For each pole ξ_j, we set $M_j = A - \Re(\xi_j)I$, and we let α_j be the eigenvalue of M_j with largest absolute value, and β_j be the eigenvalue of M_j with smallest absolute value. If $\Re(\xi_j) > 0$, then $\alpha_j < \beta_j < 0$. Moreover, we let

$$\rho_j = \gamma_j + \sqrt{\gamma_j^2 - 1} \quad \text{with} \quad \gamma_j = \frac{|\alpha_j - i\Im(\xi_j)| + |\beta_j - i\Im(\xi_j)|}{|\alpha_j - \beta_j|}. \tag{4.2}$$

The following bound holds.

THEOREM 4.3. *Assume that the spectrum of A is contained in the negative interval $[\alpha,\beta]$, and that Ψ_ν has distinct roots. Then, with the notation above,*

$$\min_{q\in\mathbb{P}_{m-1}}\max_{\lambda\in[\alpha,\beta]}\left|1-(\mathcal{R}_\nu(\lambda))^{-1}q(\lambda)\right| \le 2\sum_{j=1}^{\nu}\left(\max_{\lambda\in[\alpha,\beta]}\frac{|\tau_j|}{\mathcal{R}_\nu(\lambda)\,|\lambda-\xi_j|}\right)\frac{1}{\rho_j^m+1/\rho_j^m}.$$

Proof. In the proof we omit the polynomial subscripts. We first rewrite the problem as

$$\min_{q\in\mathbb{P}_{m-1}}\max_{\lambda\in[\alpha,\beta]}\left|1-(\mathcal{R}(\lambda))^{-1}q(\lambda)\right| = \min_{q\in\mathbb{P}_{m-1}}\max_{\lambda\in[\alpha,\beta]}\left|\frac{1}{\mathcal{R}(\lambda)}(\mathcal{R}(\lambda)-q(\lambda))\right| \qquad (4.3)$$

Let q^* be the polynomial of degree at most $m-1$ that attains the minimum in (4.3). Using the partial fraction expansion in (3.2), for any $q\in\mathbb{P}_{m-1}$ we have

$$|\mathcal{R}(\lambda)-q^*(\lambda)| = \left|\tau_0+\sum_{j=1}^{\nu}\frac{\tau_j}{\lambda-\xi_j}-q^*(\lambda)\right| \le \max_{\lambda\in[\alpha,\beta]}\left|\tau_0+\sum_{j=1}^{\nu}\frac{\tau_j}{\lambda-\xi_j}-q(\lambda)\right|.$$

We choose $q\in\mathbb{P}_{m-1}$ defined as $q(\lambda)=\tau_0+\sum_{j=1}^{\nu}\tau_j q^{(j)}(\lambda-\xi_j)$, with $\lambda\in[\alpha,\beta]$, while $q^{(j)}\in\mathbb{P}_{m-1}$, $j=1,\dots\nu$ are polynomials yet to be determined. We set $p^{(j)}(\lambda-\xi_j)=1-(\lambda-\xi_j)q^{(j)}(\lambda-\xi_j)$, with $p^{(j)}\in\mathbb{P}_m$ and $p^{(j)}(\xi_j)=1$. Thus

$$\begin{aligned}\left|\tau_0+\sum_{j=1}^{\nu}\frac{\tau_j}{\lambda-\xi_j}-q(\lambda)\right| &= \left|\sum_{j=1}^{\nu}\tau_j\left(\frac{1}{\lambda-\xi_j}-q^{(j)}(\lambda-\xi_j)\right)\right| \\ &= \left|\sum_{j=1}^{\nu}\tau_j\frac{1}{\lambda-\xi_j}p^{(j)}(\lambda-\xi_j)\right|.\end{aligned}$$

It was shown in [15, formula (38)] that the polynomial $p^{(j)}$ can be constructed so that $\max_{\zeta\in[\alpha-\xi_j,\beta-\xi_j]}|p^{(j)}(\zeta)|=2/(\rho_j^m+1/\rho_j^m)$. Hence, we can write

$$\begin{aligned}\min_{q\in\mathbb{P}_{m-1}}\max_{\lambda\in[\alpha,\beta]}\left|\frac{1}{\mathcal{R}(\lambda)}(\mathcal{R}(\lambda)-q(\lambda))\right| &\le \max_{\lambda\in[\alpha,\beta]}\left|\sum_{j=1}^{\nu}\frac{\tau_j}{\mathcal{R}(\lambda)(\lambda-\xi_j)}p^{(j)}(\lambda-\xi_j)\right| \\ &\le \sum_{j=1}^{\nu}\left(\max_{\lambda\in[\alpha,\beta]}\frac{|\tau_j|}{\mathcal{R}(\lambda)\,|\lambda-\xi_j|}\right)\frac{2}{(\rho_j^m+1/\rho_j^m)}.\end{aligned}$$ □

The denominator in the bound always satisfies $|\lambda-\xi_j|\neq 0$ if $\Im(\xi_j)\neq 0$. For ν odd and real ξ_j, we have $\xi_j>0$ for Padé, so that $\lambda-\xi_j<0$ for $\lambda\in[\alpha,\beta]$, while for Chebyshev, we have $\xi_j<0$ and $-\lambda\in[\alpha,\beta]$, so that $\lambda-\xi_j>0$. In both cases, $|\lambda-\xi_j|\neq 0$.

REMARK 4.4. When $\beta=0$, so that the eigenvalues of A are in $[\alpha,0]$, then roughly $\rho_j\approx 2(1+2|\xi_j/\alpha|)$. Therefore, we obtain

$$\sum_{j=1}^{\nu}\left(\max_{\lambda\in[\alpha,\beta]}\frac{|\tau_j|}{\mathcal{R}_\nu(\lambda)\,|\lambda-\xi_j|}\right)\frac{2}{(\rho_j^m+1/\rho_j^m)} \approx e^{-\alpha}\sum_{j=1}^{\nu}\max_{\lambda\in[\alpha,\beta]}\frac{|\tau_j|}{|\lambda-\xi_j|}\cdot\frac{2}{(2+4|\frac{\xi_j}{\alpha}|)^m},$$

which shows the role of ξ_j as $|\alpha|$ gets large. See also section 8 for additional remarks on the role of the poles. $\square$

To show the sharpness of the bound in Theorem 4.3, we next report a numerical experiment with both Padé and Chebyshev rational functions. Below and later in the paper, we show convergence curves for $\|\exp(A)v - x_m\|_*$, where $\|\cdot\|_*$ is the norm of interest. The bound $\|\exp(A)v - x_m\|_* \le \|\exp(A)v - \mathcal{R}_\nu(A)v\|_* + \|\mathcal{R}_\nu(A)v - x_m\|_*$ allows us to use estimates such as that in Theorem 4.3 to bound the second term in the right-hand side, whereas the first term depends on the accuracy of the rational function approximation. We will see that the error $\|\exp(A)v - x_m\|_*$ stagnates at the final accuracy level of $\|\exp(A)v - \mathcal{R}_\nu(A)v\|_*$.

Example 4.5. This is a contrived example but here and later in the text, it serves as a simple platform for describing the principal properties of the two rational approximations. We consider the 100×100 diagonal matrix A of the logarithm of equispaced values between 0.2 and 0.99. In Matlab notation, this can be defined as `A = diag(log(linspace(0.2,0.99,100)))`. The spectrum of A is contained in the interval $[-1.61, -0.0101]$. The vector v is chosen to be the vector of all ones, scaled so as to have unit norm. The Padé polynomials Ψ_ν, Φ_ν are computed for $\nu = 7$ and $\nu = 11$, and no pre-scaling of A is employed (see section 7). The approximate solution $x_m^G = V_m y_m^G$ is obtained at each step m by explicitly computing $V_m^* \Psi_\nu(A) V_m$ and $V_m^* \Phi_\nu(A) v$, and then solving (1.3).

In the left plot of Figure 4.1 we report the relative $\Psi_\nu(A)$-norm of the error, $\|\exp(A)v - x_m^G\|_{\Psi_\nu(A)}$ (solid black curve with squares), together with the upper bound in Theorem 4.3 corresponding to Padé rational functions with $\nu = 7, 11$. Note that the $\Psi_\nu(A)$-norm of the error is indistinguishable for the two values of ν. The right plot shows the same curves associated with Chebyshev rational functions with $\nu = 7, 14$. As predicted by the theory, the final level of accuracy is reached at about $10^{-\nu}$.

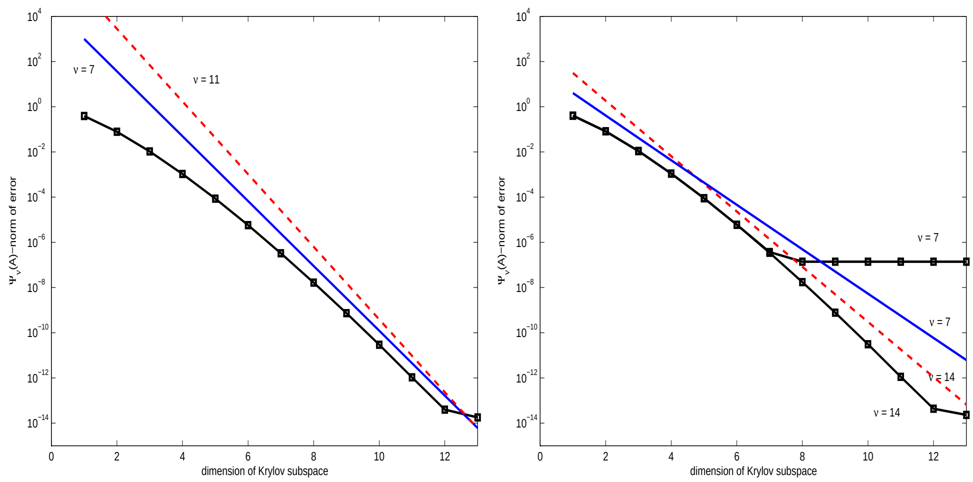

Fig. 4.1. *Example 4.5. Galerkin approximation. Left: Padé rational functions (black solid with squares) and upper bound for $\nu = 7, 11$. Right: Chebyshev rational functions (black solid with squares) and upper bounds for $\nu = 7, 14$.*

We remark that the bound is significantly accurate for the Padé approximation. The deterioration due to the high degree $\nu = 11$ is mostly noticed during the first phase of the convergence; but see also section 8. A very satisfactory bound is obtained for the Chebyshev approximation as well, especially for $\nu = 14$.

5. Layers of Galerkin approximations. The Krylov approximation in (1.4) requires the solution of the system $\Psi_\nu(H_m)y_m = \Phi_\nu(H_m)e_1$. This is interpreted in [51] as a sequential Galerkin projection onto the Krylov subspace $K_m(A, v)$ of the linear systems

$$(A - \xi_j I)w_m^{(j)} = w_m^{(j-1)}, \quad j = 1, \dots, \nu,$$

with $w_m^{(0)} = V_m y_m^{(0)}$ and $y_m^{(0)} = \Phi_\nu(H_m)e_1$. The solution of each system in the Krylov subspace then corresponds to employing the Full Orthogonalization method (FOM) [42]. Indeed, writing $w_m^{(j)} = V_m y_m^{(j)}$ for $j = 1, \dots, \nu$, we have

$$V_m^*(A - \xi_j I)V_m y_m^{(j)} = y_m^{(j-1)}, \quad j = 1, \dots, \nu,$$

that is, $(H_m - \xi_j I)y_m^{(j)} = y_m^{(j-1)}$, $j = 1, \dots, \nu$, so that, using (3.1),

$$\begin{aligned} y_m \equiv \frac{1}{\psi_\nu} y_m^{(\nu)} &= \frac{1}{\psi_\nu}(H_m - \xi_\nu I)^{-1} \cdots (H_m - \xi_1 I)^{-1}\Phi_\nu(H_m)e_1 \\ &\equiv (\Psi_\nu(H_m))^{-1}\Phi_\nu(H_m)e_1. \end{aligned}$$

In this section we try to increase our understanding of the Krylov approximation. Next result states an explicit relation between the Galerkin and Krylov solutions when the approximation subspace has dimension larger than ν. We show that the two matrices $V_m^*\Psi_\nu(A)V_m, \Psi_\nu(H_m)$, coincide except for the bottom $\nu - 1$ diagonal block. This result also allows us to conclude that the two solutions tend to coalesce as convergence takes place.

PROPOSITION 5.1. *For $m > \nu$, let $y_m^K = (\Psi_\nu(H_m))^{-1}\Phi_\nu(H_m)e_1$ and $y_m^G = (V_m^*\Psi_\nu(A)V_m)^{-1}V_m^*\Phi_\nu(A)v$ be the Krylov and Galerkin approximations to the vector $x_\star = (\Psi(A))^{-1}\Phi_\nu(A)v$, respectively. Then, there exists a $(\nu - 1) \times (\nu - 1)$ matrix S_ν, such that $V_m^*\Psi_\nu(A)V_m = \Psi_\nu(H_m) + S_{m,\nu}$, with $S_{m,\nu} = E_{m,\nu-1}S_\nu E_{m,\nu-1}^*$, and $E_{m,\nu-1}^* = [0, I_{\nu-1}] \in \mathbb{R}^{(\nu-1)\times m}$. As a consequence, $\Phi_\nu(A)v = V_m\Phi_\nu(H_m)e_1$, and*

$$y_m^K = y_m^G + (V_m^*\Psi_\nu(A)V_m)^{-1}E_{m,\nu-1}S_\nu E_{m,\nu-1}^* y_m^K,$$

so that $\|y_m^G - y_m^K\| \le \|(V_m^*\Psi_\nu(A))^{-1}E_{m,\nu-1}S_\nu\| \, \|E_{m,\nu-1}^* y_m^K\|$.

Proof. We eliminate the polynomial subscripts in the proof. For any polynomial Ψ of degree at most ν, it can be explicitly shown that for $j \le m - \nu + 1$, $V_m^*\Psi(A)V_m e_j = \Psi(H_m)e_j$ and because of symmetry, it also holds $e_j^* V_m^*\Psi(A)V_m = e_j^*\Psi(H_m)$. Therefore, we can write $S_{m,\nu} = E_{m,\nu-1}S_\nu E_{m,\nu-1}^*$, $E_{m,\nu-1}^* = [0, I_{\nu-1}]$, for some $(\nu - 1) \times (\nu - 1)$ matrix S_ν, from which the first result follows.

The fact that the two vectors $\Phi(A)v$ and $V_m\Phi(H_m)e_1$ are equal is an immediate consequence of the matrix relation above. Using the definition of y_m^K, y_m^G, we have

$$\begin{aligned} (V_m^*\Psi(A)V_m - S_{m,\nu})y_m^K &= \Phi(H_m)e_1, \\ y_m^K - (V_m^*\Psi(A)V_m)^{-1}S_{m,\nu}y_m^K &= (V_m^*\Psi(A)V_m)^{-1}\Phi(H_m)e_1 \equiv y_m^G, \\ y_m^K - y_m^G &= (V_m^*\Psi(A)V_m)^{-1}S_{m,\nu}y_m^K, \end{aligned}$$

from which the relation and the final bound follow. □

Direct inspection shows that $\|S_\nu\| = O(h_{m+1,m}^2)$. In Table 5.1, we report some numerical results that highlight the relation between the two methods. Data in Example 4.5 with the Padé rational function of degree $\nu = 7$ are considered. The columns

m	$\|x_\star - x_m^K\|$	$\|x_\star - x_m^G\|$	$\|x_\star - x_m^G\|_{\Psi_\nu}$	$\|x_m^K - x_m^G\|$
1	2.3574e-01	2.3565e-01	2.7175e-01	4.0544e-04
2	4.6261e-02	4.6749e-02	5.4550e-02	2.9431e-03
3	6.1459e-03	6.2329e-03	7.3193e-03	5.8970e-04
4	6.1599e-04	6.2576e-04	7.3762e-04	7.1273e-05
5	4.9501e-05	5.0333e-05	5.9474e-05	6.3820e-06
6	3.3163e-06	3.3738e-06	3.9931e-06	4.5871e-07
7	1.9031e-07	1.9368e-07	2.2948e-07	2.7646e-08
8	9.5430e-09	9.7134e-09	1.1518e-08	1.4367e-09
9	4.2452e-10	4.3215e-10	5.1269e-10	6.5655e-11
10	1.6955e-11	1.7261e-11	2.0484e-11	2.6769e-12
11	6.1394e-13	6.2500e-13	7.4186e-13	9.8467e-14
12	2.2013e-14	2.2331e-14	2.7469e-14	3.3028e-15
13	8.4927e-15	8.4682e-15	1.2372e-14	1.8598e-16

TABLE 5.1

Example 4.5. Convergence of Galerkin and Krylov approaches using Padé approximation with $\nu = 7$. The last column shows the difference between the two solutions.

display the norm of the error for the Krylov method, as the subspace dimension increases, and the 2-norm and Ψ_ν-norm of the error for the Galerkin method. The two approaches show very close although not identical, approximation (cf. $\|x_m^K - x_m^G\|$). We also notice that the error between the two solutions decreases with m, the difference being one order of magnitude smaller than the approximation error.

Although the result of Proposition 5.1 sheds light on the similarities of the two methods for large m, the two approaches behave very similarly even for $m \le \nu$. The analysis for $m \le \nu$ is of great interest, since for $\|A\|$ not much greater than unit, high convergence rate can be observed for the two methods, and final accuracy is obtained for m possibly smaller than ν, as is the case in Example 4.5. In the following section we show that the error in the Krylov approximation can be bounded in a way similar to what we derived for the Galerkin approximation.

5.1. The Krylov approximation. The proof of Theorem 4.3 inspires an alternative way to justify the use of the Krylov approach in (1.4) to approximate the rational function $\mathcal{R}_\nu(A)v$. Using the partial fraction expansion in (3.2) we can write

$$x_\star = \mathcal{R}_\nu(A)v = \tau_0 v + \sum_{j=1}^{\nu} \tau_j (A - \xi_j I)^{-1} v. \tag{5.1}$$

Therefore, an approximation to $x_\star$ may be obtained by approximating the solution $d^{(j)}$ to each system $(A - \xi_j I)d = v$, $j = 1, \ldots, \nu$; this type of approach has been explored for instance in [18, 5, 2, 4, 31]. Thanks to the shift invariance property of Krylov subspaces, i.e. $K_m(A, v) = K_m(A - \xi_j I, v)$ for any $\xi_j \in \mathbb{C}$, approximations to $d^{(j)}$ can be obtained in the same subspace $K_m(A, v)$ as $d_m^{(j)} = V_m y_m^{(j)}$ for some $y_m^{(j)}$ using the FOM method. More precisely, if $y_m^{(j)}$ is determined by imposing a Galerkin (orthogonality) condition on the residual $v - (A - \xi_j I)V_m y_m^{(j)}$, then we obtain

$y_m^{(j)} = (H_m - \xi_j I)^{-1} e_1$. Therefore, substituting $y_m^{(j)}$ in the expansion yields

$$\begin{aligned} x_\star &= \tau_0 v + \sum_{j=1}^{\nu} \tau_j (A - \xi_j I)^{-1} v \approx \tau_0 v + \sum_{j=1}^{\nu} \tau_j V_m y_m^{(j)} \\ &= V_m \left(\tau_0 e_1 + \sum_{j=1}^{\nu} \tau_j (H_m - \xi_j I)^{-1} e_1 \right) = V_m \mathcal{R}_\nu (H_m) e_1. \end{aligned} \tag{5.2}$$

The last term is precisely the Krylov approximation (1.4).

Theorem 4.3 shows that the approximation obtained by a Galerkin projection minimizes the error in the $\Psi(A)$-norm over all approximations in the subspace $K_m(A, v)$, and thus we expect a larger error with the Krylov approximation. The derivation above shows that the Krylov approximation yields a Galerkin solution on each system with $(A - \xi_j I)$, however, since $(A - \xi_j I)$ is not Hermitian for ξ_j complex, the Galerkin solution does not yield an error minimizing process. Note however that if for some j, ξ_j is real (and positive) then the matrix $A - \xi_j I$ is negative definite, therefore the Krylov approach does provide an error minimizing solution for that term in the expansion.

If one abandons the idea of using the Krylov approximation (5.2), the expansion in (5.1) suggests that one could use any available method for solving $(A - \xi_j I)d = v$ for each j. In particular, one could exploit the fact that $A - \xi_j I$ is normal and complex symmetric, to devise an efficient minimum residual approach (cf. [28], [16, Theorem 3.4]) that would yield a term-wise (with respect to the partial fraction expansion) optimal method for approximating $x_\star$. We refer to [35] for a discussion of a closely related approach from a polynomial point of view.

5.2. Residual and error in the Krylov approximation. We next provide a direct bound for the error of the Krylov approach in (5.2), defined as

$$e_m^K := \mathcal{R}_\nu(A)v - x_m^K = \sum_{j=1}^{\nu} \tau_j ((A - \xi_j I)^{-1} v - V_m y_m^{(j)}). \tag{5.3}$$

We can also introduce the residual vector,

$$r_m^K = \sum_{j=1}^{\nu} \tau_j (v - (A - \xi_j I) V_m y_m^{(j)}),$$

which is a linear combination of the ν residuals of the partial fraction expansion. It is remarkable that the error e_m^K and the residual r_m^K written in the expansion form, are a fully algebraic representation of the error ϵ_m and of the generalized residual ρ_m defined using the Cauchy integral form in [26, §6.3, p. 1566]; see also [22] where a similar connection is made. Denote with $r_m^{(j)}$ the residual of the jth term in the expansion. Since $r_m^{(i)} = v - (A - \xi_j I) V_m y_m^{(i)} = v - V_{m+1} H_{m+1,m} y_m^{(i)} = -v_{m+1} h_{m+1,m} e_m^* y_m^{(i)}$, we have

$$r_m^K = -v_{m+1} h_{m+1,m} \sum_{j=1}^{\nu} \tau_j e_m^* y_m^{(j)}, \qquad \text{with} \quad V_m^* r_m^K = 0, \tag{5.4}$$

and $e_m^K = -h_{m+1,m} \sum_{j=1}^{\nu} (A - \xi_j I)^{-1} v_{m+1} \tau_j e_m^* y_m^{(j)}$. Note that the Galerkin residual $r_m^G = \Phi_\nu(A)v - \Psi_\nu(A) x_m^G$ also satisfies $V_m^* r_m^G = 0$, however, r_m^G does not belong to the subspace generated by v_{m+1}.

The quantity $h_{m+1,m}|e_m^* y_m^K|$ is a well established a-posteriori estimate of the error of the Krylov approximation [26, 41, 43]. As shown in (5.2), the Krylov approximation is given by $V_m y_m^K = \tau_0 V_m e_1 + V_m \sum_{j=1}^{\nu} \tau_j y_m^{(j)}$, so that $e_m^* y_m^K = \sum_{j=1}^{\nu} \tau_j e_m^* y_m^{(j)}$ for $m > 1$, and

$$h_{m+1,m}|e_m^* y_m^K| = \left| h_{m+1,m} \sum_{j=1}^{\nu} \tau_j e_m^* y_m^{(j)} \right| = \|r_m^K\|.$$

Hence, the a-posteriori convergence estimate is precisely the norm of the residual r_m^K; see [7] for similar considerations.

We next bound the error of the Krylov approximation. We first need a lemma that bounds the error obtained when solving each system in the partial fraction expansion; see [29, formula (1.3)] for a qualitatively similar result.

LEMMA 5.2. *Let $M_j = A - \Re(\xi_j)I$, and let α_j, β_j be the largest and smallest eigenvalues of M_j in absolute value, respectively. Moreover, let $\widehat{\beta}_j = \beta_j$ if M_j is definite, which includes the case $\Im(\xi_j) = 0$, otherwise $\widehat{\beta}_j = 0$. Then, with the notation above, the error $e_m^{(j)} = (A - \xi_j I)^{-1} v - V_m(H_m - \xi_j I)^{-1} e_1$ satisfies*

$$\|e_m^{(j)}\| \le \widehat{\kappa}_j \|(A - \xi_j I)^{-1} v\| \frac{2}{\rho_j^m + 1/\rho_j^m}.$$

where $\widehat{\kappa}_j = |\alpha_j - i\Im(\xi_j)|/|\widehat{\beta}_j - i\Im(\xi_j)|$ and ρ_j is the solution to the problem in (4.2).

Proof. The proof is inspired by that of [15, Theorem 4]. Let $d_\star = (A - \xi_j I)^{-1} v$, $d_m = V_m(H_m - \xi_j I)^{-1} e_1$, $e_m^{(j)} = d_\star - d_m$, $e_0^{(j)} = d_\star$ and $r_m = (A - \xi_j I) e_m^{(j)} = M_j e_m^{(j)} - i\Im(\xi_j) e_m^{(j)}$. In the following we will omit the superscript in the error, and we will use $\langle u, v \rangle = u^* v$. We have $\langle r_m, e_m \rangle = \langle M_j e_m, e_m \rangle - \langle i\Im(\xi_j) e_m, e_m \rangle$, so that

$$|\langle r_m, e_m \rangle|^2 = (\langle M_j e_m, e_m \rangle)^2 + \Im(\xi_j)^2 (\langle e_m, e_m \rangle)^2 \ge (\widehat{\beta}_j^2 + \Im(\xi_j)^2)\|e_m\|^4.$$

We also have $\|r_m\|^2 = \|M_j e_m\|^2 + \Im(\xi_j)^2 \|e_m\|^2 \le (\alpha_j^2 + \Im(\xi_j)^2)\|e_m\|^2$. Recalling that $r_m \perp K_m(M_j, v)$, for any $u \in K_m(M_j, v)$ we have

$$\begin{aligned} |\langle r_m, e_m \rangle|^2 &= |\langle r_m, d_\star - u \rangle|^2 \\ &\le \|r_m\|^2 \, \|d_\star - u\|^2 \le (\alpha_j^2 + \Im(\xi_j)^2)\|e_m\|^2 \, \|d_\star - u\|^2. \end{aligned}$$

Collecting all bounds, we obtain $(\widehat{\beta}_j^2 + \Im(\xi_j)^2)\|e_m\|^4 \le (\alpha_j^2 + \Im(\xi_j)^2)\|e_m\|^2 \, \|d_\star - u\|^2$, that is

$$\|e_m\|^2 \le \frac{\alpha_j^2 + \Im(\xi_j)^2}{\widehat{\beta}_j^2 + \Im(\xi_j)^2} \, \|d_\star - u\|^2.$$

Since u is arbitrary, we take as u the solution to the problem

$$\min_{u \in K_m} \|d_\star - u\| = \min_{p \in \mathbb{P}_m, p(0)=1} \|p(A - \xi_j I) e_0\|.$$

Therefore, arguing as in the proof of Theorem 4.3, we have

$$\min_{p \in \mathbb{P}_m, p(0)=1} \|p(A - \xi_j I) e_0\| \le \|e_0\| \, \frac{2}{\rho_j^m + 1/\rho_j^m},$$

and the final result follows. $\square$

In the lemma above, for ν odd, $M_j = A - \Re(\xi_j)I$ is negative definite for the real (positive) Padé pole, whereas in the case of the real (negative) Chebyshev pole, $M_j = -A - \Re(\xi_j)I$ is positive definite (we recall here the change of sign in the case of Chebyshev function). This ensures that the lemma holds for both Chebyshev and Padé rational functions. Moreover, for definite M_j, a sharper bound can be obtained; see Lemma 7.1.

THEOREM 5.3. *Assume the previous notation holds, and that the poles ξ_j are distinct. Let $M_j = A - \Re(\xi_j)I$ and α_j, β_j be the largest and smallest eigenvalues of M_j in absolute value, respectively. Then, with the notation of Lemma 5.2,*

$$\|e_m^K\| \le 2\sum_{j=1}^{\nu} \left(|\tau_j|\widehat{\kappa}_j\|(A-\xi_j I)^{-1}v\|\right)\frac{1}{\rho_j^m + 1/\rho_j^m}.$$

Proof. Using the definition of e_m^K in (5.3) and its partial fraction representation, we have

$$\|e_m^K\| \le \sum_{j=1}^{\nu}|\tau_j|\|e_m^{(j)}\|, \qquad e_m^{(j)} = (M_j - i\Im(\xi_j)I)^{-1}v - V_m y_m^{(j)}. \tag{5.5}$$

From Lemma 5.2, it follows $\|e_m^{(j)}\| \le 2\widehat{\kappa}_j\|(A-\xi_jI)^{-1}v\|/(\rho_j^m + 1/\rho_j^m)$. Substituting in (5.5), the result follows. $\square$

For $\widehat{\kappa}_j \approx 1$, we have

$$|\tau_j|\widehat{\kappa}_j\|(A-\xi_jI)^{-1}v\| \approx |\tau_j|\|(A-\xi_jI)^{-1}v\| \le \max_{\lambda\in[\alpha,\beta]}\frac{|\tau_j|}{|\lambda-\xi_j|},$$

where the last term is precisely the factor in the bound of the Galerkin approach; see Remark 4.4. The condition $\widehat{\kappa}_j \approx 1$ is met for instance when $[\alpha,\beta]\approx[-1,0]$. Indeed, in this case, the poles in the partial fraction expansion are significantly larger in absolute value than the values in $[-1,0]$, so that $\widehat{\kappa}_j = |(\alpha-\xi_j)/(\beta-\xi_j)| \approx |\xi_j|/|\xi_j| = 1$.

Roughly speaking, the result of Theorem 5.3 tells us that the convergence rate of the bound is driven by the convergence of the single systems $(A-\xi_jI)d = v$, $j = 1,\ldots,\nu$ with the FOM method. We also explicitly observe that the convergence rate of systems with matrix $A-\xi_jI$ is significantly different from that observed with A. This is due to the fact that the spectrum of $A-\xi_jI$ is in a complex line segment near ξ_j, sufficiently far away from the origin to ensure fast convergence. These observations should be compared to those in [24] and earlier literature, where the rate of convergence of iterative solvers for systems with A was observed to be an unsatisfactory tool for describing the convergence rate in the exponential approximation.

Finally, we have experimented with the bounds for the Krylov approximation as in Example 4.5, and numerical results almost identical to those of Figure 4.1 were obtained.

6. Some computational advantages of rational function approximation. The use of rational functions and their partial fraction expansion allows us to exploit and generalize known properties of Krylov subspace methods for the solution of algebraic linear systems. In particular, in this section we show that our formulation makes it easy to interpret recently proposed strategies.

As an immediate consequence of our formulation, in the following proposition we provide a bound for the components of the solution y_m^K. Analyzing the pattern of the solution components is of interest when using some recently developed preconditioning strategies [49]. In these promising techniques, the Krylov subspace with respect to the matrix $(I-\gamma A)^{-1}$ is generated, for a conveniently chosen scalar γ. An approximation to $\exp(A)$ is then obtained in this rational space. Since $(I-\gamma A)^{-1}$ cannot be applied exactly, it is shown that the accuracy with which the inverse needs to be employed can be tied to the magnitude of the solution components in the generated Krylov subspace; we refer to [49, section 5] for a more comprehensive discussion.

Proposition 6.1. *Assume the notation of the previous sections holds. Let $x_m^K = V_m y_m^K$ be the Krylov approximation to the exponential operator and assume that for $k \le m$, the matrix $H_k - \xi_j I$ is nonsingular for all poles ξ_j, $j = 1, \ldots, \nu$. Then*

$$|e_k^* y_m^K| \le |e_k^* e_1 \tau_0| + \sum_{j=1}^{\nu} \frac{|\tau_j|}{\sigma_{\min}(H_m - \xi_j I)} \|r_{k-1}^{(j)}\|, \qquad k \le m,$$

where $\sigma_{\min}(H_m - \xi_j I)$ is the smallest singular value of $H_m - \xi_j I$, and $\|r_{k-1}^{(j)}\|$ is the residual norm associated with the jth partial fraction expansion system in $K_{k-1}(A, v)$.

Proof. Using the partial fraction expansion of $\mathcal{R}_\nu(H_m)$ we have

$$y_m^K = \tau_0 e_1 + \sum_{j=1}^{\nu} \tau_j (H_m - \xi_j I)^{-1} e_1 = \tau_0 e_1 + \sum_{j=1}^{\nu} \tau_j y_m^{(j)}, \tag{6.1}$$

from which

$$e_k^* y_m^K = e_k^* e_1 \tau_0 + \sum_{j=1}^{\nu} \tau_j e_k^* y_m^{(j)}. \tag{6.2}$$

It was shown in [46, Lemma 5.2] that if the matrix $H_k - \xi_j I$ is nonsingular for all $k = 1, \ldots, m$, so that the residuals $r_{k-1}^{(j)}$ are well defined, then

$$|e_k^* y_m^{(j)}| \le |e_k^* e_1 \tau_0| + \frac{1}{\sigma_{\min}(H_m - \xi_j I)} \|r_{k-1}^{(j)}\|.$$

Substituting in (6.2), the result follows. □

The result of Proposition 6.1 shows that the components of y_m^K approximately decrease with the residuals of the shifted systems in the expansion. This fact can be exploited to rigorously show that the preconditioning technique proposed in [49] can be successfully implemented with an *inexact* application of $(I-\gamma A)^{-1}$ and a *relaxed* tolerance [40].

If convergence is not fast, a problem encountered with Krylov subspace approximation is that the maximum allowed approximation space dimension is limited by memory restrictions, and thus some form of restarting must be devised. We next show that our rational function framework provides a simple though effective way to describe a recently proposed restarting strategy. Once the vector $x_m^K = \tau_0 v + \sum_{j=1}^{\nu} V_m y_m^{(j)}$ is determined, a new approximation space can be obtained as $K_m(A, v_{m+1})$ with $v_{m+1} = V_{m+1} e_{m+1}$ and associated matrix $V_m^{(1)}$, so that the approximation can be updated as

$$x_m^K = (\tau_0 v + \sum_{j=1}^{\nu} V_m y_m^{(j)}) + \sum_{j=1}^{\nu} V_m^{(1)} (y_m^{(j)})^{(1)}, \tag{6.3}$$

with obvious notation for $(y_m^{(j)})^{(1)}$. We rewrite (6.3) as $x_m^K = \tau_0 v + \sum_{j=1}^{\nu} \Big(V_m y_m^{(j)} + V_m^{(1)} (y_m^{(j)})^{(1)} \Big)$. Recalling that this approach approximates $\tau_0 v + \sum_{j=1}^{\nu} (A - \xi_j I)^{-1} v$, this relation shows that each term in the expansion formula is nothing but the approximate solution obtained by restarted FOM applied to each shifted system separately. This last statement can be verified by recalling that all systems residuals $r_m^{(j)}$ are collinear with v_{m+1} (cf. (5.4)), so that the method can be restarted with the same approximation space for all systems [45]. Further use of the properties of the restarted FOM method, see, e.g., [44], shows that this restarting procedure corresponds to Algorithm 2 in [14] when used with rational functions; see also [27] for more results on the derivation of the restarted approximation method.

Finally, appropriate Krylov subspace approaches and rational function approximations can be used to preserve geometric properties of the exponential of skew-symmetric matrices; this is the subject of current investigation [30].

7. The role of $\|A\|$ in the Padé approximation. In the previous sections we assumed that $\|A\|$ was not much greater than unit. For the case of Chebyshev rational functions, this is an unnecessary constraint, as good approximations to e^{-x} can be obtained for $x \in [0, +\infty)$; see, e.g., [8]. In the right plot of Figure 7.1 we report the convergence curve and its bound, for the Krylov approximation using Chebyshev rational functions with $\nu = 14$, for the matrix in Example 7.3. In the plot, the ideal bound (2.1) is also reported.

Padé rational function approximation is effective for $\|A\|$ close to the origin. Otherwise, a procedure called scaling and squaring is commonly employed in conjunction with Padé functions, that allows one to compute an approximation to the exponential of a conveniently scaled matrix; see, e.g., [21]. The procedure amounts to finding the smallest integer $s \geq 0$ such that $\|A\|_\infty / 2^s$ is less than a prescribed value, a common value being 1/2. Recent work by Higham has shown that this latter value can be significantly relaxed, depending on the rational function degree used in the approximation [23]. For the sake of simplicity, here we limit ourselves to the case $\|A\|_\infty 2^{-s} \leq \frac{1}{2}$. Setting $\widetilde{A} = A/2^s$, the scaling and squaring method produces the matrix $B = (\mathcal{R}_\nu(\widetilde{A}))^{-1}$, so that the sought after approximation is obtained as $\exp(A) \approx B^{2^s}$, where the operation is performed by repeated squaring of B. Within the Krylov approximation (1.2), scaling and squaring can be conveniently performed at each step m as $\exp(H_m) e_1 \approx (\mathcal{R}_\nu(H_m/2^s))^{2^s} e_1$, where s may vary with m [43].

We next show that this corrected scheme can be included in our theoretical analysis. Let $s \geq 0$ be the smallest integer such that $\widetilde{A} := A/2^s$ satisfies $\|\widetilde{A}\| \leq 1/2$. The construction of the Krylov subspace $K_m(\widetilde{A}, v)$ corresponds to scaling H_m in (1.1) by the quantity 2^s, independent of m but dependent on $\|A\|$. Since $\|H_m\| \leq \|A\|$ for all $m \geq 0$, this approach is more conservative than the one that scales H_m by a different quantity at each iteration. We then approximate $\exp(A)v$ as

$$\exp(A)v \approx \Big(\mathcal{R}_\nu(\widetilde{A})\Big)^{2^s} v \approx V_m \Big(\mathcal{R}_\nu(\widetilde{H}_m)\Big)^{2^s} e_1 \equiv V_m y_m^K.$$

In the scaling and squaring method, the Padé approximant has poles of multiplicity 2^s, so that the partial fraction expansion is given by

$$\mathcal{R}_\nu(\zeta)^{2^s} = \widetilde{\tau}_0 + \sum_{j=1}^{\nu} \sum_{\ell=1}^{2^s} \frac{\widetilde{\tau}_{j,\ell}}{(\zeta - \xi_j)^\ell}, \tag{7.1}$$

where $\xi_1, \ldots, \xi_\nu$ are the roots of Ψ_ν and

$$\widetilde{\tau}_{j,\ell} = \frac{1}{(\ell-1)!} \frac{d^{\ell-1}}{(d\zeta)^{\ell-1}} \frac{(\zeta-\xi_j)^{2^s}\Phi_\nu(\zeta)^{2^s}}{\Psi_\nu(\zeta)^{2^s}}\bigg|_{\zeta=\xi_j}.$$

Therefore, we can write

$$\left(\mathcal{R}_\nu(\widetilde{A})\right)^{2^s} v = \widetilde{\tau}_0 v + \sum_{j=1}^{\nu}\sum_{\ell=1}^{2^s} \widetilde{\tau}_{j,\ell}(\widetilde{A}-\xi_j I)^{-\ell} v.$$

Because of the multiple poles, the computation of $\widetilde{\tau}_{j,\ell}$ may be very ill conditioned, therefore, we do not advocate implementing this procedure. Instead, it provides a way to theoretically justify this computational strategy within our polynomial framework. Once again, setting $x_\star = \mathcal{R}_\nu(\widetilde{A})^{2^s} v$, we use the bound

$$\|\exp(A)v - V_m y_m^K\| \le \|\exp(A)v - x_\star\| + \|x_\star - V_m y_m^K\|,$$

in which the magnitude of the first term depends on the accuracy of the rational approximation, whereas only the second term depends on the accuracy in the Krylov subspace. By approximating each inverse power in the Krylov subspace, we have

$$\begin{aligned} x_\star &= \widetilde{\tau}_0 v + \sum_{j=1}^{\nu}\sum_{\ell=1}^{2^s} \widetilde{\tau}_{j,\ell}(\widetilde{A}-\xi_j I)^{-\ell} v \\ &\approx \widetilde{\tau}_0 v + \sum_{j=1}^{\nu}\sum_{\ell=1}^{2^s} \widetilde{\tau}_{j,\ell} V_m(\widetilde{H}_m-\xi_j)^{-\ell} e_1 = V_m \left(\mathcal{R}_\nu(\widetilde{H}_m)\right)^{2^s} e_1. \end{aligned}$$

In spite of the presence of multiple poles, we next show that the error can be bounded similarly to what we did for the simple poles. In fact, the bound for the error in practice is not influenced by the presence of the scaling and squaring method.

We first derive a bound for the errors in the partial fraction expansion, which holds for symmetric and definite matrices.

LEMMA 7.1. *Let $M_j = A - \Re(\xi_j)I$ be a symmetric definite matrix, and let α_j, β_j be the largest and smallest eigenvalues of M_j in absolute value, respectively, so that $\kappa_j = \alpha_j/\beta_j > 0$ is the condition number of M_j. Then, the error $e_m^{(j)} = (A-\xi_j I)^{-1}v - V_m(H_m-\xi_j I)^{-1}e_1$ satisfies*

$$\|e_m^{(j)}\| \le \kappa_j^{\frac12}\eta_j\|(A-\xi_j I)^{-1}v\| \frac{2}{\rho_j^m + 1/\rho_j^m}.$$

where $\eta_j = \left(1 + \frac{\Im(\xi_j)^2(\kappa_j-1)^2}{4\kappa_j\Im(\xi_j)^2+\alpha_j^2(\kappa_j+1)^2}\right)^{\frac12}$, and ρ_j is the solution to the problem in (4.2).

Proof. We assume that M_j is positive definite, otherwise we can work with $-M_j$. For each $j = 1, \ldots, \nu$, $y_m^{(j)}$ is computed by imposing a Galerkin condition on the corresponding residual $v - (M_j - i\Im(\xi_j)I)V_m y_m^{(j)}$. It was shown in [15, Theorem 4] that if M_j is definite, then

$$\|e_m^{(j)}\|_{M_j} \le 2\frac{\eta_j}{\rho_j^m + \frac{1}{\rho_j^m}}\|e_0^{(j)}\|_{M_j}.$$

Then $\|e_m^{(j)}\| \le \|M_j^{-1/2}\| \|e_m^{(j)}\|_{M_j}$, $\|e_0^{(j)}\|_{M_j} \le \|M_j^{1/2}\| \|e_0^{(j)}\|$, where $\|M_j^{1/2}\|$ denotes the norm of $M_j^{1/2}$, induced by the vector 2-norm, and $\|e_0^{(j)}\| = \|(A - \xi_j I)^{-1} v\|$. $\square$

The bound of Lemma 7.1 is analogous to that in Lemma 5.2 for $\widehat{\kappa}_j \approx 1$, which is the case when $\|A\| \le 1$. The new bound of Lemma 7.1 provides a sharper estimate for $\|A\| > 1$ and M_j definite, therefore it can be used with Padé rational functions.

THEOREM 7.2. *With the notation and definitions of Lemma 7.1, let ξ_j, $j = 1, \ldots, \nu$ be the roots of $\Psi_\nu(\lambda)$. Assume that the eigenvalues of A are contained in $[\alpha, \beta]$, and that $\frac{1}{2^s} \frac{|\lambda|}{|\xi_j|} \ll 1$ for $\lambda \in [\alpha, \beta]$. Let $x_\star = \left(\mathcal{R}_\nu(\widetilde{A})\right)^{2^s} v$ and $y_m^K = \left(\mathcal{R}_\nu(\widetilde{H}_m)\right)^{2^s} e_1$. Finally, for $j = 1, \ldots, \nu$, let*

$$\widehat{\tau}_j := \max_{\ell=1,\ldots,2^s} \frac{|\widetilde{\tau}_{j,\ell}|}{|(-\xi_j)^{\ell-1}|}.$$

Then

$$\|x_\star - V_m y_m^K\| \,\tilde{\le}\, 2^{s+1} \sum_{j=1}^{\nu} |\widehat{\tau}_j| \kappa_j^{\frac{1}{2}} \frac{\eta_j}{\rho_j^m + \frac{1}{\rho_j^m}} \|(A - \xi_j I)^{-1}\|.$$

where $\tilde{\le}$ means that higher order terms are omitted.

Note that the bound is in terms of A and not of its scaled counterpart $\widetilde{A}$.

Proof. Recalling (7.1), we have

$$\begin{aligned} R_{2^s}(\lambda) := \left(\mathcal{R}_\nu(\frac{\lambda}{2^s})\right)^{2^s} &= \widetilde{\tau}_0 + \sum_{j=1}^{\nu} \sum_{\ell=1}^{2^s} \frac{\widetilde{\tau}_{j,\ell}}{(\frac{\lambda}{2^s} - \xi_j)^\ell} \\ &= \widetilde{\tau}_0 + \sum_{j=1}^{\nu} \sum_{\ell=1}^{2^s} \frac{\widetilde{\tau}_{j,\ell}}{\xi_j^\ell (\frac{\lambda}{2^s \xi_j} - 1)^\ell}. \end{aligned}$$

For $\frac{|\lambda|}{2^s |\xi_j|} \ll 1$, we have $(\frac{\lambda}{2^s \xi_j} - 1)^\ell \approx (-1)^\ell (\frac{\ell}{2^s \xi_j} \lambda - 1)$, so that

$$R_{2^s}(\lambda) \approx \widetilde{\tau}_0 + \sum_{j=1}^{\nu} \sum_{\ell=1}^{2^s} \frac{\widetilde{\tau}_{j,\ell}}{(-\xi_j)^\ell (\frac{\ell\lambda}{2^s \xi_j} - 1)} = \widetilde{\tau}_0 - \sum_{j=1}^{\nu} \sum_{\ell=1}^{2^s} \frac{\widetilde{\tau}_{j,\ell}}{(-\xi_j)^{\ell-1} (\frac{\ell}{2^s} \lambda - \xi_j)}.$$

Let $\omega_{j,\ell} := \widetilde{\tau}_{j,\ell} / (-\xi_j)^{\ell-1}$. Then,

$$\begin{aligned} \|x_\star - V_m y_m^K\| &= \|R_{2^s}(A) v - V_m R_{2^s}(H_m) e_1\| \\ &\approx \| \sum_{j=1}^{\nu} \sum_{\ell=1}^{2^s} \omega_{j,\ell} \left((\frac{\ell}{2^s} A - \xi_j I)^{-1} v - V_m (\frac{\ell}{2^s} H_m - \xi_j I)^{-1} e_1 \right) \| \\ &\le \sum_{j=1}^{\nu} \sum_{\ell=1}^{2^s} |\omega_{j,\ell}| \|\epsilon_{j,\ell}\|, \end{aligned}$$

where $\epsilon_{j,\ell} = (\frac{\ell_j}{2^s} A - \xi_j I)^{-1} v - V_m (\frac{\ell_j}{2^s} H_m - \xi_j I)^{-1} e_1$. Note that the approximation above is ensured to hold for H_m because the eigenvalues of $H_m = V_m^T A V_m$ are also contained in $[\alpha, \beta]$, so that $\frac{|\theta|}{2^s |\xi_j|} \ll 1$ for any eigenvalue θ of H_m. Using Lemma 7.1 and appropriately modifying the notation, we have

$$\|\epsilon_{j,\ell}\| \le 2 \left(\kappa(\frac{\ell}{2^s} A - \Re(\xi_j) I) \right)^{\frac{1}{2}} \frac{\eta_{j,\ell}}{\rho_{j,\ell}^m + \frac{1}{\rho_{j,\ell}^m}} \|(\frac{\ell}{2^s} A - \xi_j I)^{-1} v\|.$$

Since $\ell/2^s \le 1$ for $\ell \in \{1,\dots,2^s\}$, we have $\|(\ell_j/2^s A - \xi_j I)^{-1}\| \le \|(A-\xi_j I)^{-1}\|$ and

$$\kappa(\frac{\ell_j}{2^s}A - \Re(\xi_j)I)\eta_{j,\ell}^2 \le \kappa(A-\Re(\xi_j)I))\eta_{j,2^s}^2 \equiv \kappa_j\eta_j^2; \tag{7.2}$$

see the appendix for a proof of this inequality. From the definition of $\rho_{j,\ell}$, it follows that

$$\frac{|\frac{\ell}{2^s}\alpha - \Re(\xi_j) - i\Im(\xi_j)| + |\frac{\ell}{2^s}\beta - \Re(\xi_j) - i\Im(\xi_j)|}{\frac{\ell}{2^s}|\alpha-\beta|} = \frac{|\alpha - \frac{2^s}{\ell}\xi_j| + |\beta - \frac{2^s}{\ell}\xi_j|}{|\alpha-\beta|} \ge \frac{|\alpha-\xi_j| + |\beta-\xi_j|}{|\alpha-\beta|},$$

from which it follows that $\rho_{j,\ell} \ge \rho_{j,2^s} > 1$, and because of monotonicity, we obtain

$$\frac{1}{\rho_{j,\ell}^m + \frac{1}{\rho_{j,\ell}^m}} \le \frac{1}{\rho_{j,2^s}^m + \frac{1}{\rho_{j,2^s}^m}}.$$

Since $\rho_{j,2^s}$ corresponds to the convergence with $(A-\xi_j I)$, we can set $\rho_{j,2^s} = \rho_j$. Collecting all bounds, we obtain

$$\|\epsilon_{j,\ell}\| \le 2\kappa_j^{\frac12}\frac{\eta_j}{\rho_j^m + \frac{1}{\rho_j^m}}\|(A-\xi_j I)^{-1}\|.$$

Since $|\omega_{j,\ell}| \le |\widehat{\tau}_j|$, we finally have

$$\begin{aligned}\sum_{j=1}^{\nu}\sum_{\ell=1}^{2^s}|\omega_{j,\ell}|\|\epsilon_{j,\ell}\| &\le 2\sum_{j=1}^{\nu}\sum_{\ell=1}^{2^s}|\widehat{\tau}_j|\kappa_j^{\frac12}\frac{\eta_j}{\rho_j^m + \frac{1}{\rho_j^m}}\|(A-\xi_j I)^{-1}\| \\ &\le 2\cdot 2^s\sum_{j=1}^{\nu}|\widehat{\tau}_j|\kappa_j^{\frac12}\frac{\eta_j}{\rho_j^m + \frac{1}{\rho_j^m}}\|(A-\xi_j I)^{-1}\|. \qquad \square\end{aligned}$$

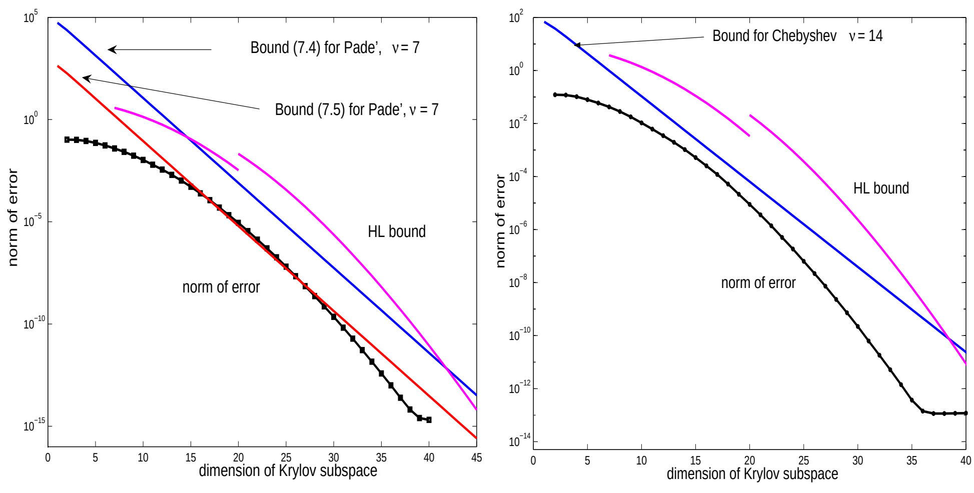

FIG. 7.1. *Example 7.3 with $\|A\| \gg 1$, Krylov approximation. Left. Padé rational function with scaling and squaring: convergence curve and upper bound for $\nu = 7$, and ideal bound. Right. Chebyshev rational function: convergence curve and upper bound for $\nu = 14$, and ideal bound.*

A few remarks are in order. We first notice that the bound in Theorem 7.2 fully mimics the bound in Theorem 5.3. The only relevant difference is the presence of the additional scaling factor 2^s. The two bounds also differ for the terms $\widehat{\tau}_j$'s. In our experiments, however, replacing $\widehat{\tau}_j$ with τ_j did not seem to affect the approximation.

Although the approximation $V_m y_m^K$ with Padé does require scaling and squaring, the convergence rate does not seem to depend on it. The proof suggests that one could use the following estimate

$$\|x_\star - V_m y_m^K\| \approx \|\mathcal{R}_\nu(A)v - V_m \mathcal{R}_\nu(H_m)e_1\|, \tag{7.3}$$

where however, for $\|A\| \gg 1$, neither $\mathcal{R}_\nu(A)v$ is a good approximation to $x_\star$, nor $V_m\mathcal{R}_\nu(H_m)e_1$ is a good approximation of $V_m y_m^K$.

Example 7.3. We consider the 1001×1001 diagonal matrix A in [24] with entries uniformly distributed in $[-40, 0]$, and the random vector v with uniformly distributed values in $[0, 1]$ (Matlab function `rand`) and unit norm. In Figure 7.1 we report the convergence of the error norm for the Krylov method, together with the ideal bound (2.1) from [24] (referred to as HL bound). In the plot, we also report the following estimate, derived from Theorem 7.2 by replacing $\widehat{\tau}_j$ with τ_j, the latter being the coefficients in the partial fraction expansion of $\mathcal{R}_\nu(\lambda)$,

$$\|x_\star - V_m y_m^K\| \mathrel{\tilde{\le}} 2^{s+1} \sum_{j=1}^{\nu} |\tau_j| \frac{\kappa_j}{\rho_j^m + \frac{1}{\rho_j^m}} \|(A - \xi_j I)^{-1}\|. \tag{7.4}$$

$$\|x_\star - V_m y_m^K\| \mathrel{\tilde{\le}} 2 \sum_{j=1}^{\nu} |\tau_j| \frac{\kappa_j}{\rho_j^m + \frac{1}{\rho_j^m}} \|(A - \xi_j I)^{-1}\| \tag{7.5}$$

The new bound for the error norm does not significantly differ from those observed in previous sections, although in this case the actual Padé approximation is performed with scaling and squaring. In other words, convergence seems to be only driven by the spectral properties of the matrix, as stressed by the bound on the convergence rate that is based on polynomial estimates of the shifted spectrum of A.

8. Recovering superlinear convergence. Our bounds for both Galerkin and Krylov approximations with rational functions of degree ν predict *linear* convergence as the Krylov subspace dimension m increases. The superlinear convergence expressed, say, in the first bound of Theorem 2.1 can be recovered as a function of the degree of the rational function. To explain this approach, we first recall that the bounds in Theorem 2.1 were determined in two steps in [24, Theorem 2]. In the first step, the error is bounded by means of the Cauchy integral on a curve Γ, which is the boundary of a piecewise smooth bounded region containing the numerical range of A. The second step amounts to conveniently choosing Γ so as to appropriately bound the Cauchy integral. In particular, the selected curve is a parabola whose right-most point turns out to be equal to $\gamma = m^2/(4\rho)$, in the notation of Theorem 2.1 (cf. [24, pp. 1916-1917]). Therefore, the chosen curve moves away from the spectrum with m^2, as the Krylov subspace dimension m increases.

The partial fraction expansion of $\mathcal{R}_\nu$ may be viewed as a way to approximate the Cauchy integral representation of $\exp(\lambda)$ for a fixed integration curve passing through the expansion poles. It is known that in both cases of Padé and Chebyshev approximations $\mathcal{R}_\nu$, the poles ξ_j tend to infinity as ν increases. Therefore, a larger degree ν corresponds to selecting a curve Γ that is farther away from the spectrum. In other words, we expect better approximation of the bounds with small ν at an early convergence stage, whereas larger ν are required to appropriately bound the convergence curve as the dimension of the Krylov subspace increases. For the Chebyshev approximation, superlinear convergence as ν increases may be observed in the right plot of Figure 4.1, where the straight line for $\nu = 7$ better represents the early convergence stage, whereas the line for $\nu = 14$ sharply bounds the convergence curve for larger m.

In the case of Padé approximation, this behavior can be better formalized, yielding a relation between the approximation degree and the dimension of the Krylov subspace. Using [1, Theorem 5.7.3], we know that the poles of the Padé approximant $\mathcal{R}_\nu$ of degree ν are located in the complex annulus[2]

$$2 \cdot 0.27\nu \le |z| \le 2\nu + \frac{4}{3}.$$

Therefore, if we wish to employ poles on a curve that intersects the positive real semi-axis close to the "optimal value" $m^2/(4\rho)$, we require that ν satisfies $2 \cdot 0.27\nu \le \frac{m^2}{4\rho} \le 2\nu + \frac{4}{3}$, that is

$$\frac{m^2}{8\rho} - \frac{2}{3} \le \nu \le \frac{1}{0.27}\frac{m^2}{8\rho}. \tag{8.1}$$

Hence, if the degree ν is chosen within the bounds above, we expect that the Padé rational function approximates the Cauchy integral on a quasi-optimal curve, with respect to m, in the sense of [24]. For instance, below are the values of ν satisfying the lower bound in (8.1) for $m \in \{1, \dots, 40\}$ and $\rho = 10$,

m	4	8	12	16	20	24	28	32	36	40
ν	0	1	2	3	5	7	10	13	16	20

The fidelity of this correspondence can be fully appreciated in Figure 8.1 for the data in Example 7.3. Reported are the actual error curve (solid with squares), and the ideal bounds of Theorem 2.1. We also display the upper bounds in (7.4) for the Padé approximation with ρ_j associated with the poles for $\nu = 1, 4, 7, 10, 14, 18$. Remarkably, the envelope of the reported straight lines completely reproduces the true convergence history, while the single lines well represent the local convergence behavior at the corresponding subspace dimension m (e.g., the line for $\nu = 7$ well approximates the convergence slope around iteration $m = 24$).

Finally, we stress that all reported bounds, included the ideal bounds, only depend on the spectral interval of the given matrix, and not on the location of the eigenvalues within this interval. Particular eigenvalue distributions may cause severe overestimations of the true convergence behavior; see, e.g., [10, §3.2].

9. Conclusions and outlook. We have proposed a new analysis of Krylov subspace methods for approximating the action of matrix rational functions with specific application to the matrix exponential operator. We have shown a minimization property of one of the methods, we have provided new upper bounds for the approximation error by using partial fraction expansion, and we have theoretically justified some computational strategies.

[2]It is also possible to detect a parabolic region that is pole-free; see [1, Theorem 5.7.4]. This would more closely mimic the choice of the curve Γ in [24]. However, for the sake of simplicity we limit our presentation to this more intuitive case.

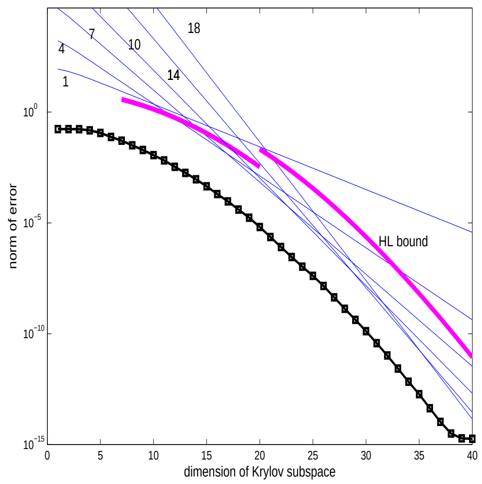

FIG. 8.1. *Example 7.3. Krylov approximation with Padé rational function. Bound in* (7.4) *for* $\nu = 1, 4, 7, 10, 14, 18$. *The ideal bounds of Theorem 2.1 are also reported (labelled "HL bound").*

Our analysis may be generalized to cases in which the rational function employed to approximate the exponential is different from the widely used Padé or Chebyshev, as in [38, 3]. Among these generalizations, the case of polynomial approximation of the exponential is particularly appealing for its simplicity; see, e.g., [11]. We also refer to [14, 35] for examples of polynomial interpolation at points different from the eigenvalues of H_m. Without great differences, one could extend our results to the case of *restricted denominator* (RD) rational forms, which are rational functions $R_{j,k} = \frac{q_j(x)}{(1+\rho x)^k}$ where $\rho \in \mathbb{R}$ and q_j is a polynomial of degree not greater than j. Such RD-rational forms have been introduced in [37] and recently used to approximate the exponential of a matrix in [34]. Our theoretical results may provide some insight into the selection of the parameters involved in the definition of the RD-rational form.

Some of our results may be naturally extended to the case of non-Hermitian A, although optimality results of the Galerkin method do not carry over. Finally, the techniques and the analysis used in this paper could be adapted to the numerical approximation of other analytic functions in the Krylov subspace, such as $A^{\frac{1}{2}}$; see [13, 53] and references therein.

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Appendix. We prove inequality (7.2) in the proof of Theorem 7.2.

Proof. Let $\xi_j = \xi_R + i\xi_I$ and $\kappa_{j,\ell} = \kappa(\frac{\ell}{2^s}A - \xi_j I)$. We have

$$\kappa_{j,\ell}\eta_{j,\ell}^2 = \kappa_{j,\ell} + \kappa_{j,\ell}\frac{\xi_I^2(\kappa_{j,\ell}-1)^2}{4\kappa_{j,\ell}\xi_I^2 + (\frac{\ell}{2^s}\alpha - \xi_R)(\kappa_{j,\ell}+1)^2}.$$

Let $\chi = \ell/2^s$ and $\kappa_{j,\ell} = (\chi\alpha - \xi_R)/(\chi\beta - \xi_R) =: f(\chi)$. Since $\alpha < \beta < 0$ and $\xi_R > 0$, we have $f'(\chi) = \xi_R(-\alpha+\beta)/(\chi\beta - \xi_R)^2 > 0$, that is, f is a monotonically increasing function, so that $\kappa_{j,\ell} = f(\chi) \le f(1) = \kappa_{j,2^s}$ for $\chi \in (0, 1]$. With analogous reasoning, we have that $\sqrt{f(\chi)}+1/\sqrt{f(\chi)} \geq \sqrt{f(1)}+1/\sqrt{f(1)}$ and that $(\chi\alpha - \xi_R) \geq (\alpha - \xi_R)$ for $\chi \in (0,1]$. Therefore,

$$\begin{aligned}\kappa_{j,\ell}\eta_{j,\ell}^2 &= \kappa_{j,\ell} + \kappa_{j,\ell}\frac{\xi_I^2(\kappa_{j,\ell}-1)^2}{\kappa_{j,\ell}\left(4\xi_I^2 + (\frac{\ell}{2^s}\alpha - \xi_R)(\sqrt{\kappa_{j,\ell}} + \frac{1}{\sqrt{\kappa_{j,\ell}}})^2\right)} \\ &\leq \kappa_{j,2^s} + \frac{\xi_I^2(\kappa_{j,2^s}-1)^2}{4\xi_I^2 + (\alpha - \xi_R)(\sqrt{\kappa_{j,2^s}} + \frac{1}{\sqrt{\kappa_{j,2^s}}})^2} = \kappa_j\eta_j^2. \qquad \square\end{aligned}$$

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