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Krylov subspace methods for functions of fractional differential operators

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Abstract

The paper deals with the computation of functions of fractional powers of differential operators. The spectral properties of these operators naturally suggest the use of rational approximations. In this view we analyze the convergence properties of the shift-and-invert Krylov method applied to operator functions arising from the numerical solution of differential equations involving fractional diffusion.

1 Introduction

Problems involving fractional powers of differential operators arise in various fields of applications. As a model we can consider the space fractional Bloch-Torrey equation involving the two dimensional fractional Laplacian operator:

$$\begin{aligned}
\frac{\partial}{\partial t}y(t,x) &= -K_\alpha(-\Delta)^{\alpha/2}y(t,x)+F(t,y(t)), \quad t>t_0, \quad x\in\Omega, \qquad (1.1)\\
y(t,x) &= 0, \quad x\in\partial\Omega,\\
y(t_0,x) &= y_0(x),
\end{aligned}$$

where K_α is a positive real parameter depending only on α, Ω is a bounded domain and the linear operator $(-\Delta)^{\alpha/2}$, with $1<\alpha\leq 2$, can be defined through the eigenfunction expansion of the standard Laplacian by raising the eigenvalues to the fractional power $\alpha/2$. In this sense, the fractional Laplacian is identified with the fractional power of the classical Laplacian with Dirichlet boundary conditions (cf. [23, Definition 1]). In other words, the operator $(-\Delta)^{\alpha/2}$ plays the role of a fractional differential operator (see [38, 39, 4, 40]). Such type of models have been widely considered in describing the phenomenon of the anomalous diffusion in various scientific areas. In the sequel we will consider also the time-fractional counterpart of (1.1) where $\frac{\partial}{\partial t}y(t,x)$ is replaced by a fractional Caputo's derivative. Concerning the spatial discretization of the Laplacian, with

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homogeneous Dirichlet boundary conditions, classical finite differences lead to a banded or block banded matrix A whose power $A^{\alpha/2}$ is an approximation to $(-\Delta)^{\alpha/2}$. This procedure, called "matrix transfer technique", was proposed in [22, 23]. We remark that the fractional Laplace operator is alternatively defined using the Fourier transform on an infinite domain [35]. Using such definition and assuming to work with homogeneous Dirichlet boundary conditions, in [38, Lemma 1] it has been proved that the definition used in the present paper is equivalent to the Riesz fractional derivative, so that other kinds of discretization are possible (see e.g. [33]).

Depending on the method used to solve (1.1), the approximate solution can be expressed through functions of the standard Laplacian. We refer in particular to functions $f(x)$, for $x > 0$, like $(1+tx^c)^{-1}$ or $\exp(-tx^c)$, $t > 0$, and similar ones, where $1/2 < c \leq 1$ and assuming to work with the standard branches of these functions. The presence of singularities as well as of branch cuts may affect the performance of any approximation method. For the treatment of some functions involving $(-\Delta)^{\alpha/2}$, the use of the Standard (polynomial) Krylov Method (SKM) has been investigated in [39]. As it is well known such procedure presents some drawbacks in dealing with discretizations of differential operators. In this paper we consider in alternative the one-pole rational method usually called the shift-and-invert Krylov Method (SIKM). We develop a convergence theory assuming to work more generally with positive self-adjoint linear operators acting on suitable Hilbert spaces. The convergence theory embraces the case of functions that can be represented either in the Stieltjes integral form or in a more general Dunford-Taylor form.

The paper is organized as follows. In Section 2 we give an outline of some widely used Krylov methods. In Section 3 we present a convergence analysis for the SIKM. In Section 4 we discuss some cases related to problems like (1.1) giving some hints about the proper choice of the pole. Practical a posteriori error bounds that can be used to arrest the process are discussed in Section 5. The results of some numerical experiments are reported in Section 6 .

2 Krylov approximations

Let $\mathbb{X}$ be a (separable) Hilbert space endowed with the scalar product $\langle \cdot, \cdot \rangle$ and norm $\|\cdot\|$, and let A be a positive self-adjoint closed linear operator with dense domain $\mathbb{D}(A) \subseteq \mathbb{X}$ and spectrum $\sigma(A) \subset [a, +\infty)$, for $a > 0$. Moreover we assume that A has compact inverse. Since in practice we deal with discretizations of differential operators, this turns out to be a realistic framework in order to investigate the features of the SIKM. As mentioned, the fractional powers of A can be defined by considering the orthonormal basis of eigenvectors $u_k \in \mathbb{X}$ corresponding to eigenvalues $\lambda_k^2 > 0$, $k = 1, 2, \ldots$. Then, for $\frac{1}{2} < c < 1$, the fractional power A^c is a self adjoint positive linear operator defined as

$$A^c v = \sum_{k=1}^{\infty} \lambda_k^{2c} b_k u_k,$$

for any $v = \sum_{k=1}^{\infty} b_k u_k \in \mathbb{D}(A^c)$, with $\mathbb{D}(A) \subseteq \mathbb{D}(A^c) \subseteq \mathbb{X}$, where

$$\mathbb{D}(A^c) = \left\{ v = \sum_{k=1}^{\infty} b_k u_k : \sum_{k=1}^{\infty} \lambda_k^{2c} |b_k|^2 < +\infty \right\}.$$

As it is well known, other definitions can be adopted (see [10, 27]).

From now on let Π_k denote the set of the algebraic polynomials of degree less or equal than k. We recall that $\mathcal{K}_k(T, v) = \{p(T)v, p \in \Pi_{k-1}\}$ indicates the k-th Krylov subspace associated with a linear operator T and a vector v. Projections on such subspaces are widely used dealing with functions of large matrices. For the computation of

$$y = f(A)v,$$

these procedures produce approximations of the type $\overline{y} = R_{i,j}(A)v$, where $R_{i,j}$ is a rational function, i.e., $R_{i,j} = \frac{p_i}{q_j}$, $p_i \in \Pi_i$, $q_j \in \Pi_j$. More precisely, for $k \geq 1$, let $\mathcal{K}_k$ be a subspace of dimension k associated to a rational function of A and let $V_k : \mathbb{C}^k \to \mathcal{K}_k$ be a linear operator, such that $V_k^* V_k = I_k$ (the identity in $\mathbb{C}^k$), where V_k^* denotes the adjoint of V_k. Then

$$\overline{y} = V_k f(B_k) V_k^* v, \tag{2.1}$$

can be taken as an approximation in $\mathcal{K}_k$ to y, provided that $B_k \in \mathbb{C}^{k \times k}$ is suitably defined.

Dealing with matrices, commonly used approaches are the Standard Krylov Method (SKM), the Extended Krylov Method (EKM) and the the shift-and-invert Krylov method (SIKM), often called restricted-denominator Arnoldi method. These procedures belong to the class of the rational Krylov methods ([2, 17, 7, 8]).

The SKM yields polynomial approximations by projecting the problem onto the classical Krylov spaces $\mathcal{K}_k(A, v)$. The EKM works on spaces generated both by A and A^{-1}, producing rational approximations where $q_j(x) = x^j$, and $i > j$, usually $i = 2j$. The third method, the SIKM, gives one (repeated)-pole rational approximations with $i \leq j$, projecting the problem onto the Krylov spaces associated to the resolvent

$$Z = (\delta I + A)^{-1}, \tag{2.2}$$

where δ is a suitable parameter.

In the matrix case, for functions like those we are interested in, the convergence of the SKM may depend dramatically on the conditioning of the matrix A (see e.g. [5, 6, 39]). In fact, denoting by $\lambda_{\min}$ and $\lambda_{\max}$ respectively its minimum and its maximum eigenvalue, for the approximations in $\mathcal{K}_k(A, v)$ an error like $\exp\left(-2k\sqrt{\frac{\lambda_{\min}}{\lambda_{\max}}}\right)$ may occur. A better behavior can be expected from the EKM, introduced by Druskin and Knizhnerman in [6] (see also [26] for extensions). Since the approximations are sought in $\mathcal{K}_{2k}(A, A^{-k}v)$, that is,

$j = k$, $i = 2k$, an $O\left(\exp\left(-2k\sqrt[4]{\frac{\lambda_{\min}}{\lambda_{\max}}}\right)\right)$ error can be predicted. If A represents a discretization of an unbounded operator, then the convergence of both these methods may degenerate as the discretization is improved. This reflects the fact that if A is just the underlying unbounded operator then both the Standard and the Extended Krylov subspaces can be defined only for sufficiently regular data, as it occurs for any super-diagonal ($i > j$) rational function of A. Moreover, even if they are well defined, a loss of regularity occurs with respect to v.

The third approach, the SIKM, does not suffer of such drawbacks. Up from the early papers [29] and [37] concerning the matrix exponential, various applications have been discussed in literature. However, few existing results apply to our context.

In order to describe the SIKM, for a given $v \in \mathbb{X}$ and Z as in (2.2), let $\mathcal{K}_k = \mathcal{K}_k(Z, v)$, $k \geq 1$. By the Arnoldi (Lanczos) algorithm we can build up an orthonormal sequence $\{v_j\}_{j\geq 1}$, such that for each k, $\mathcal{K}_k(Z, v) = span\{v_1, v_2, ..., v_k\}$, $v_1 = v/\|v\|$. Let V_k be represented by the matrix whose columns are such basis vectors. Setting $H_k = V_k^* Z V_k$ it holds that

$$ZV_k = V_k H_k + h_{k+1,k} v_{k+1} (V_k^* v_k)^*, \tag{2.3}$$

where $h_{k+1,k} = v_{k+1}^* Z v_k > 0$. Under our assumptions H_k is tridiagonal Hermitian. In the original formulation of the SIKM, the matrix B_k in (2.1) is taken as

$$B_k = H_k^{-1} - \delta I. \tag{2.4}$$

This corresponds to the SKM applied to the problem rewritten as $y = u(Z)v$, where $u(z) = f(z^{-1} - \delta)$. Observe that in the matrix case $\sigma(B_k) \subseteq [\lambda_{\min}, \lambda_{\max}]$.

An often adopted alternative to (2.4) is

$$B_k = V_k^* A V_k. \tag{2.5}$$

This formula is commonly used for defining rational Krylov methods. See [2] for an implementation. It can be seen that both (2.4) and (2.5) satisfy

$$\|y - \overline{y}\| \leq 2\|v\| \min_{p_{k-1}\in\Pi_{k-1}} \max_{z\in\sigma(Z)\cup\sigma((\delta I + B_k)^{-1})} |u(z) - p_{k-1}(z)|. \tag{2.6}$$

As a matter of fact, the two approaches give very similar results. Observe that (2.4) avoids applications of A. Yet, it requires the use of H_k^{-1}. In this respect, in the self-adjoint case the situation simplifies, since H_k is Hermitian and tridiagonal. Thus, if k is not very large, the method can be easily implemented by means of the eigendecomposition. We point out that if A is an operator, in order to use (2.5) we must require that $\mathcal{K}_k \subset \mathbb{D}(A)$. On the other hand, (2.4) can be used anyway, even if $v \notin \mathbb{D}(A)$. In both cases, if defined, the approximations possess at least the same regularity as v.

The SIKM, as well as the EKM, has the computational advantage that all the linear systems to be solved share the same coefficient matrix. We notice that for functions like those here considered, multi-pole rational approximations have been proposed in [20, 18, 19].

3 A convergence analysis of the SIKM

In this section we will examine the convergence of the SIKM for functions related to evolution problems like (1.1). Clearly, if $u(z) = f(z^{-1} - \delta)$ is continuous in $[0, \frac{1}{\delta+a}]$ then (2.6) ensures the convergence as $k \to +\infty$. At first let us consider the matrix case. In order to estimate the rate of convergence some classical results of approximation theory can be employed, involving the well known inverse Zhukovski function

$$\Phi(\omega) = \omega + \sqrt{\omega^2 - 1}, \quad \omega \geq 1. \tag{3.1}$$

Proposition 3.1 *Assume that* $\sigma(A) \subset [a, b]$. *For any given* $\delta \geq 0$ *assume that* $u(z) = f(z^{-1} - \delta)$ *is analytic for* $0 < \Re z < \delta^{-1}$ *and continuous in* $[0, \delta^{-1}]$. *Then for every integer* $k \geq 1$

$$\min_{p_{k-1} \in \Pi_{k-1}} \max_{z \in \sigma(Z) \cup \sigma((\delta I + B_k)^{-1})} |u(z) - p_{k-1}(z)| \leq 2M \frac{\rho^k}{1 - \rho}, \tag{3.2}$$

where $M = \max_{z \in [0, \delta^{-1}]} |u(z)|$ *and*

$$\rho = \max\left(\frac{\sqrt{\delta + b} - \sqrt{\delta + a}}{\sqrt{\delta + b} + \sqrt{\delta + a}}, \frac{\sqrt{b(\delta + a)} - \sqrt{b(\delta + a)}}{\sqrt{b(\delta + a)} + \sqrt{b(\delta + a)}} \right).$$

Proof 3.2 *We can see that* $\sigma(Z) \cup \sigma((\delta I + B_k)^{-1}) \subset [(\delta + b)^{-1}, (\delta + a)^{-1}]$. *Then, by a well-known bound given in [9] concerning Faber series, we realize that*

$$\min_{p_{k-1} \in \Pi_{k-1}} \max_{z \in [(\delta+b)^{-1}, (\delta+a)^{-1}]} |u(z) - p_{k-1}(z)| \leq 2M \frac{\Phi(\omega)^{-k}}{1 - \Phi(\omega)^{-1}},$$

where

$$\omega = \min\left(\frac{2\delta + b + a}{b - a}, \frac{b(\delta + a) + a(\delta + b)}{b(\delta + a) - a(\delta + b)} \right).$$

This gives the bound.

In order to simplify the notation, from now on we will replace the current index k with $m + 1$, for $m \geq 1$. Namely, setting $Z = (\delta I + A)^{-1}$, $\delta \geq 0$, and referring to the notation of the previous section, let us consider the approximation to $y = f(A)v$ given by

$$\overline{y} = V_{m+1} f(B_{m+1}) V_{m+1}^* v, \tag{3.3}$$

with $B_{m+1} = H_{m+1}^{-1} - \delta I$ or $B_{m+1} = V_{m+1}^* A V_{m+1}$.

Optimizing the bound (3.2) by choosing $\delta = \sqrt{ab}$, by (2.6) we get

$$\|y - \overline{y}\| \leq 2M \sqrt[4]{\frac{b}{a}} \exp\left(-2m \sqrt[4]{\frac{a}{b}} \right) \|v\|. \tag{3.4}$$

Observe that, for $\delta = \sqrt{ab}$ the condition number of $\delta I + A$ is raised to $1/2$ with respect to $\frac{b}{a}$. Anyhow, as $b \to +\infty$ (for a fixed a) the bound becomes meaningless. In order to deal with this situation we resort to some integral representations. In the sequel we will denote by C any positive constant independent of the parameters involved.

At first we consider functions that can be represented in a Stieltjes integral form

$$f(x) = \int_0^\infty g(\lambda)(\lambda + x)^{-1} d\lambda, \quad x > 0, \tag{3.5}$$

where $g(\lambda)$ is such that the integral is absolutely convergent. The results stated below extend directly, with the obvious changes, to more general Stieltjes (Markov) formulations. The treatment of such cases by rational Krylov methods has been already considered in the literature. Among the others, we quote [6, 26, 28, 31, 1, 2, 18, 19, 13]. We also quote the recent thesis [36], where new results on polynomial and extended Krylov approximations to Stieltjes functions are given. In particular in [36], as well as in [31, 13], restarted procedures have been analyzed.

In the matrix case, error bounds for the SIKM can be found in [28, 31]. In particular in [28] (see also [2, Section 6]) it was shown that, assuming $\sigma(A) \subset [a, b]$, $\delta = \sqrt{ab}$, $B_{m+1} = H_{m+1}^{-1} - \delta I$, then for $\overline{y}$ defined by (3.3) we have

$$\|y - \overline{y}\| \le C \exp\left(-2m\sqrt[4]{\frac{a}{b}}\right). \tag{3.6}$$

We notice that such bound holds even for the EKSM, as shown in [6, 26]. Anyhow, the crucial issue is that the bound degenerates as the spectrum enlarges. As mentioned, this is the situation we want to analyze in view to applications involving differential operators. In [28] it was observed that the rate of convergence of the SIKM actually turns out to be independent of the size of the spectrum, provided that the parameter δ is properly chosen. The results given below will clarify more precisely this point.

We point out that not all the functions of our interest can be represented by a form (3.5). Simple examples are $\exp(-x^c)$ with $\frac{1}{2} < c \le 1$, and more generally the Mittag-Leffler functions $E_\beta(-x^c)$, for $\frac{\beta}{2} + c \ge 1$ (see Section 4). In order to treat these cases, we resort to a suitable Dunford-Taylor representation. Precisely, for any $\vartheta \in (0, \frac{\pi}{2}]$ let us consider the open sector

$$\Sigma_\vartheta = \{\lambda \in \mathbb{C} : \lambda = r\exp(i\varphi) : r \in (0, \infty), |\varphi| < \vartheta\}, \tag{3.7}$$

and let Γ_ϑ denote its boundary. Let us assume that $f(\lambda)$ is analytic in $\mathbb{C}^+ = \{\lambda : \Re\lambda > 0\}$ and continuous on $\Gamma_{\frac{\pi}{2}} = i\mathbb{R}$ with $|f(\lambda)| \to 0$ as $|\lambda| \to \infty$ for $\Re\lambda \ge 0$. Under these assumptions $y = f(A)v$ can be represented in the Dunford-Taylor form

$$y = \frac{1}{2\pi i} \int_{\Gamma_\vartheta} f(\lambda)(\lambda I - A)^{-1} v d\lambda, \tag{3.8}$$

for any $\vartheta \in (0, \frac{\pi}{2}]$. Accordingly, the approximation (3.3) can be represented in the same way. In order to simplify our analysis, below we will refer to $\vartheta = \frac{\pi}{2}$.

We point out that analogous results could be obtained for other choices of ϑ. Since we have supposed the function f to be analytic in $\mathbb{C}_+$, the analysis, with the appropriate changes, could be carried out also for sectorial operators.

For $\lambda \notin [a, \infty)$ we define the function

$$\omega(\lambda) = \frac{\delta + 2a + |a - \lambda|}{|\delta + \lambda|}, \tag{3.9}$$

and for $p > 1$, $q = \frac{p}{p-1}$, we set

$$\begin{aligned} c_p &= \Gamma(2(q-1))^{\frac{1}{q}}, \\ \overline{c}_p &= \Gamma(2(2q-1))^{\frac{1}{q}}, \end{aligned}$$

where Γ is the Gamma function. Moreover let Φ be defined by (3.1).

Now, referring to (3.3), we give some convergence results for the SIKM whose proofs are reported in the Appendix.

Proposition 3.3 *Assume $\sigma(A) \subset [a, +\infty)$, for $a > 0$. Let $v \in \mathbb{X}$. For any given $\delta \geq 0$ and $m \geq 1$ take $\mathcal{K}_{m+1} = \mathcal{K}_{m+1}(Z, v)$, $B_{m+1} = H_{m+1}^{-1} - \delta I$. For some $p > 1$ and for any $R \geq \delta$, if y is defined by (3.5) assume that*

$$s_p = \left(\int_R^\infty |g(\lambda)|^p \, d\lambda \right)^{\frac{1}{p}} < \infty, \tag{3.10}$$

and set

$$S_m(R) = \int_0^R |g(\lambda)| \, (\lambda + a)^{-1} \Phi(\omega(-\lambda))^{-m} d\lambda \,;$$

if y is defined by (3.8) with $\vartheta = \frac{\pi}{2}$ then assume that

$$s_p = \left(\int_R^\infty (|f(ir)| + |f(-ir)|)^p \, dr \right)^{\frac{1}{p}} < \infty, \tag{3.11}$$

and set

$$S_m(R) = \int_0^R \frac{|f(ir)| + |f(-ir)|}{\sqrt{a^2 + r^2}} \Phi(\omega(ir))^{-m} dr.$$

Then in both cases we have

$$\|y - \overline{y}\| \leq C \, \|v\| \, (S_m(R) + K_m(R)), \tag{3.12}$$

with

$$K_m(R) = c_p s_p(R) (qm)^{-\frac{2}{p}} (\delta + a)^{-\frac{1}{p}}.$$

The results below show that the rate of convergence of the SIKM can improve with the regularity of the data, as it was pointed out for entire functions in [16].

Proposition 3.4 *Assume $\sigma(A) \subset [a, +\infty)$, for $a > 0$.Let $v \in \mathbb{D}(\mathbb{A})$. For any given $\delta \geq 0$ and $m \geq 1$ take $\mathcal{K}_{m+1} = \mathcal{K}_{m+1}(Z, v)$ and $B_{m+1} = V_{m+1}^* A V_{m+1}$. Then in both cases, defining s_p as before and respectively*

$$\begin{aligned}
\overline{S}_m(R) &= \int_0^R |g(\lambda)| \, (\lambda + a)^{-2} \Phi(\omega(-\lambda))^{-m} d\lambda, \\
\overline{S}_m(R) &= \int_0^R \frac{|f(ir)| + |f(-ir)|}{a^2 + r^2} \Phi(\omega(ir))^{-m} dr,
\end{aligned}$$

we have

$$\|y - \overline{y}\| \leq C \, \|(A - aI)v\| \, (\overline{S}_m(R) + \overline{K}_m(R)), \tag{3.13}$$

where

$$\overline{K}_m(R) = c_p s_p(R)(qm)^{-\frac{2(p+1)}{p}} (\delta + a)^{-\frac{p+1}{p}}.$$

It is also interesting to observe that, as stated below, for regular data the convergence occurs under weaker assumptions on g and f.

Proposition 3.5 *With the notation of Propositions 3.4, assume that $|g(\lambda)| \leq M$ for all $\lambda \geq R$ in (3.5) or $|f(ir)| + |f(-ir)| \leq M$ for all $r \geq R$ in (3.8). Then we have*

$$\|y - \overline{y}\| \leq C \, \|(A - aI)v\| \left(\overline{S}_m(R) + \frac{Mm^{-2}}{\delta + a} \right). \tag{3.14}$$

Remark 3.6 *For $R \gg \delta + a$, in the previous bounds we can take $C \approx 4$ (see the proofs in the Appendix).*

The value of a can be any in the interval $(0, \lambda_{\min}]$ where $\lambda_{\min}$ stands for the minimum eigenvalue of A. Thus, as expected, the bounds depend on $\lambda_{\min}$. Nevertheless, we observe that referring to the differential operators of our interest, this value remains uniformly bounded from below independently of the quality of the discretization.

We notice that, for the implementation of the formulae, in evaluating $S_m(R)$ (or $\overline{S}_m(R)$) by means of any composite quadrature rule, one can exploit the behavior of the function ω. For instance, dealing with (3.5) we observe that $\omega(-\lambda)$ is increasing for $\lambda \in [0, \delta]$ and decreasing for $\lambda \in [\delta, R]$. Analogously, referring to (3.8), assuming without loss of generality $\delta > 2a$, one verifies that $\omega(\lambda)$ is increasing in $\left[0, \sqrt{\delta(\delta - 2a)}\right]$ and decreasing in $\left[\sqrt{\delta(\delta - 2a)}, R\right]$. The value of R should be taken sufficiently large, depending on the behavior of g or f.

In summary, the above formulas say that the error can be bounded as

$$\|y - \overline{y}\| \leq C\rho_R^m + C_R m^{-c},$$

for some $0 < \rho_R < 1$ and $c > 0$, where the coefficients C and C_R depend on g or f. Moreover $\rho_R \to 1$ and $C_R \to 0$ as $R \to \infty$. Thanks to the above observations, considering (3.5) we have

$$\rho_R = \max \left\{ \Phi(\omega(0))^{-1}, \Phi(\omega(-R))^{-1} \right\},$$

whereas for (3.8), for $\delta > 2a$,

$$\rho_R = \max\left\{\Phi(\omega(0))^{-1}, \Phi(\omega(iR))^{-1}\right\}.$$

Since this holds for any operator with spectrum in $[a, +\infty)$, this means that when the spectrum of A enlarges to infinity, a sublinear convergence term may appear. Anyway, the rate of convergence cannot become arbitrarily slow.

As it was frequently observed, a priori bounds for Krylov methods often turn out to be unreasonably rather pessimistic and this occurs also for the bounds developed in this section. This is mainly due to the so-called adaptivity of the methods to the spectrum. For discussions on this point we refer to [24, 25, 1].

4 Parameter selection and applications

Even if pessimistic, the a priori error bounds could give us some suggestions about the choice of the parameter δ. For instance, one could minimize the bounds for some suitable value of m and R, or one could simply balance the two factors in ρ_R. For some specific functions, it is also possible to adopt values already proposed in the literature (see [29, 37, 28, 32]. Referring to the matrix case, the accuracy is also affected by the conditioning of $\delta I + A$. Thus, in choosing the parameter δ, this issue should be taken into consideration. From this point of view, a too small value of δ might be inconvenient. As observed, if $\sigma(A) \subset [a, b]$, the choice $\delta = \sqrt{ab}$ allows to improve considerably the conditioning with respect to the one of A. Indeed, Z can be viewed as a common preconditioner for all the shifted matrices involved in the integral representations (see also [37]). In this respect, referring to the Stieltjes formula, one can see that taking $\delta = \sqrt{ab}$, the spectral condition number of all the preconditioned matrices $Z(\lambda I + A) = (\lambda - \delta)Z + I$ (as well as that of $\delta I + A$) is less or equal to $\sqrt{b/a}$, which can be reached at $\lambda = 0$ and for $\lambda \to \infty$.

In some cases a suitable choice of the parameter is suggested by the particular function involved, as it occurs in those we consider below. As already mentioned they concern functions related to numerical methods for solving initial value problems of type (1.1) or their time-fractional counterparts. Without loss of generality we set $K_\alpha = 1$, for any for $1 < \alpha < 2$.

Example 4.1 *In classical implicit one-step methods the solution of systems like $(I + tA^{\frac{\alpha}{2}})y = v$, for some $t > 0$, is required. By obvious reasons the computation of $A^{\frac{\alpha}{2}}$ should be avoided. The function $f(x) = (1 + tx^{\frac{\alpha}{2}})^{-1}$ is analytic with a cut on the negative real axis. Accordingly (see [11, 27]), it can be represented in the form (3.5) where*

$$g(\lambda) = -\frac{\Im f(\lambda e^{i\pi})}{\pi}, \tag{4.1}$$

namely

$$g(\lambda) = \frac{t \sin(\frac{\pi\alpha}{2})}{\pi} \left(\frac{\lambda^{\frac{\alpha}{2}}}{1 + 2t\lambda^{\frac{\alpha}{2}} \cos\left(\frac{\pi\alpha}{2}\right) + t^2\lambda^\alpha} \right). \tag{4.2}$$

Clearly all the results in Section 3 apply. Note that $|g(\lambda)|$ *takes its maximum at* $\lambda^* = t^{-\frac{2}{\alpha}}$. *It seems reasonable to pick just* $\delta = \lambda^*$, *even more when* α *is close to* 2. *The aim of this choice is to minimize the error component corresponding to the values of* λ *close to* λ^*. *This appears more evident looking at the equivalent formula*

$$f(x) = \frac{\sin(\frac{\pi\alpha}{2})}{\pi} \int_0^\infty \left(\frac{\lambda^{\frac{\alpha}{2}}}{1 + 2\lambda^{\frac{\alpha}{2}} \cos\left(\frac{\pi\alpha}{2}\right) + \lambda^\alpha} \right) (\lambda + t^{\frac{2}{\alpha}} x)^{-1} d\lambda.$$

Example 4.2 *The exponential-like functions called* φ*-functions are defined by*

$$\begin{aligned} \varphi_0(z) &= \exp(z), \\ \varphi_k(z) &= \frac{\varphi_{k-1}(z) - \varphi_{k-1}(0)}{z}, \quad \varphi_k(0) = \frac{1}{k!}, \quad k \geq 1. \end{aligned}$$

As it is well known, they represent the core of the modern exponential integrators (see [21] for a review). In order to apply such methods for solving (1.1), one has to compute

$$y_k(t) = t^k \varphi_k(-tA^{\frac{\alpha}{2}})v, \quad t > 0,$$

for some given v *and for some (small) values of* k. *Here we focus the attention on* $\varphi_0(-tA^{\frac{\alpha}{2}}) = \exp(-tA^{\frac{\alpha}{2}})$ *which is the analytical semigroup having* $A^{\frac{\alpha}{2}}$ *as its infinitesimal generator. Considering* $\exp\left(-tx^{\frac{\alpha}{2}}\right)$, *if* $\alpha = 1$ *then it has the Stieltjes representation (3.5) with*

$$g(\lambda) = \frac{\sin(t\sqrt{\lambda})}{\pi}.$$

Clearly the assumptions of Proposition 3.3 do not hold. But, if $v \in \mathbb{D}(A)$ *(or if* A *is a matrix), then Proposition 3.5 applies and the convergence occurs. As an alternative one could also use the function* $f(x) = \frac{1-\exp(-t\sqrt{x})}{x}$ *, which can be represented (cf. [6]) as*

$$f(x) = \frac{1}{\pi} \int_0^{+\infty} \frac{\sin(t\sqrt{\lambda})}{\lambda} (\lambda + x)^{-1} d\lambda, \quad x > 0. \tag{4.3}$$

For $1 < \alpha < 2$ *we realize that* $|g(\lambda)|$ *cannot be bounded in* $[0, \infty)$ *(see also Example 4.3 below), since for* $x > 0$, *we obtain (see [11, 27])*

$$\exp\left(-x^{\frac{\alpha}{2}}\right) = \frac{1}{\pi} \int_0^\infty \frac{\exp\left(-\lambda^{\frac{\alpha}{2}} \cos\left(\frac{\alpha\pi}{2}\right)\right)}{\lambda + x} \sin\left(\lambda^{\frac{\alpha}{2}} \sin\left(\frac{\alpha\pi}{2}\right)\right) d\lambda.$$

Therefore no result of Section 3 relative to the representation (3.5) can be used for this form. Nevertheless we can resort to (3.8), with $f(\lambda) = \exp(-t\lambda^{\frac{\alpha}{2}})$, *since* $\left|\exp(-t\lambda^{\frac{\alpha}{2}})\right| \leq \exp(-tr^{\frac{\alpha}{2}} \cos(\frac{\alpha}{2}\vartheta))$, *for* $t > 0$ *and for* $|\vartheta| \in (0, \frac{\pi}{2}]$. *Similar considerations can be made for the functions* φ_k *for* $k \geq 1$. *Even in this case for small* t *a choice like* $\delta = t^{-\frac{2}{\alpha}}$ *seems reasonable.*

Example 4.3 *The above observations can be extended to the generalized Mittag-Leffler (ML) functions depending on two positive real parameters β, γ. They are defined by the series expansion*

$$E_{\beta,\gamma}(z) = \sum\nolimits_{k=0}^{\infty} \frac{z^k}{\Gamma(\beta k+\gamma)}, \quad z \in \mathbb{C}, \tag{4.4}$$

where Γ denotes the gamma function. For $0 < \beta \leq 1$ and $1 < \alpha < 2$, they are closely related to the fractional differential problem

$$\begin{gathered} {}_0D_t^{\beta} y(t) + K_{\alpha} A^{\frac{\alpha}{2}} y = F(t), \ t \in [0,T], \\ y(0) = y_0, \end{gathered} \tag{4.5}$$

where $K_\alpha > 0$ and ${}_0D_t^{\beta} u(t)$ denotes the Caputo's fractional derivative of order β (cf. [34]). Setting $K_\alpha = 1$, the solution to (4.5) can be expressed as

$$y(t) = E_{\beta,1}(-t^{\beta} A^{\frac{\alpha}{2}}) y_0 + \int_0^t (t-s)^{\beta-1} E_{\beta,\beta}(-A^{\frac{\alpha}{2}}(t-s)^{\beta}) F(s) ds.$$

In particular, for $k = 0, 1, \ldots$, we have

$$\int_0^t (t-s)^{\beta-1} E_{\beta,\beta}(-(t-s)^{\beta} A^{\frac{\alpha}{2}}) s^k ds = t^{\beta+k} E_{\beta,\beta+k+1}(-t^{\beta} A^{\frac{\alpha}{2}}).$$

Arguing as in [39, Proposition 4.4], it can be seen that $E_{\beta,\gamma}(-t^{\beta} A^{\frac{\alpha}{2}})$ has the Stieltjes representation (3.5) with

$$g(\lambda) = -\frac{\Im E_{\beta,\gamma}(-t^{\beta} \lambda^{\frac{\alpha}{2}} \exp(\frac{i\alpha\pi}{2}))}{\pi}.$$

We recall that (cf. [34, Theorem 1.6]) if $\frac{\pi\beta}{2} < \arg(z) < \pi$ then it is

$$|E_{\beta,\gamma}(z)| \leq \frac{C}{1+|z|}. \tag{4.6}$$

Therefore, as pointed out in [39] where the use of the SKM has been discussed, we have

$$|g(\lambda)| \leq \frac{C}{1+t^{\beta}\lambda^{\frac{\alpha}{2}}},$$

provided that $\alpha + \beta < 2$. Otherwise we have to adopt the representation (3.8) with $f(\lambda) = E_{\beta,\gamma}(-t^{\beta}\lambda^{\frac{\alpha}{2}})$. In fact, since $\frac{\alpha}{2} + \beta < 2$, from (4.6) we get

$$|f(\lambda)| \leq \frac{C}{1+t^{\beta}|\lambda|^{\frac{\alpha}{2}}}.$$

Thus the corresponding results stated in Section 3 can be applied. We point out that the computation of ML functions, of scalar as well as of matrix argument, has been recently addressed by various authors. See among the others [30, 15, 14, 39].

Observe that, due to (2.6), in all the three cases, for every δ and m the error vanishes as the parameter t goes to zero.

5 A posteriori error estimates

An important issue in the application of any approximation method is of course the a posteriori error evaluation. An often adopted stopping criterium for Krylov methods for $f(A)v$ is based on the norm of the so called generalized residual. Referring to the previous notations, this is given by

$$r_{m+1} = h_{m+2,m+1} \left|< e_{m+1}, f(B_{m+1})V_{m+1}^* v >\right|.$$

A similar residual-based estimator has been used in [19]. Unfortunately, similarly to what happens for linear systems, it has been observed that in many cases this error-estimate turns out to be unreasonably optimistic. Thus it is reasonable to have at disposal some suitable a posteriori error bound for a check.

Employing the SIKM with $B_{m+1} = H_{m+1}^{-1} - \delta I$ or $B_{m+1} = V_{m+1}^* A V_{m+1}$, for $\lambda \notin [a. + \infty)$, let us set

$$D(\lambda) = (\lambda I - A)^{-1} - V_{m+1}(\lambda I - B_{m+1})^{-1} V_{m+1}^*. \tag{5.1}$$

Observe that by the triangle inequality

$$\|D(\lambda)\| \le \frac{2}{dist(\lambda, [a, \infty))}. \tag{5.2}$$

In this way we can express the error in the approximation of (3.5) and (3.8) in the following forms respectively

$$y - \overline{y} = -\int_0^\infty g(\lambda) D(-\lambda) v d\lambda, \tag{5.3}$$

$$y - \overline{y} = \frac{1}{2\pi i} \int_{\Gamma_\vartheta} f(\lambda) D(\lambda) v d\lambda. \tag{5.4}$$

By the theory before developed, we have to evaluate something like

$$\|y - \overline{y}\| = \left\| \int_\Gamma \psi(\lambda) D(\lambda) v d\lambda \right\|,$$

for some contour Γ and a suitable function ψ. A well known result (see [3]) concerning the GMRES and the FOM applied to the linear system

$$((\lambda + \delta)^{-1} I - Z)x = v,$$

yields the inequality

$$\min_{p_m \in \Pi_m} \left\| \frac{p_m(Z)v}{p_m((\lambda + \delta)^{-1})} \right\| \le \mu_m(\lambda),$$

where, for $m \ge 1$ the non increasing sequence $\{\mu_m(\lambda)\}$ is defined by

$$\mu_m(\lambda) = \frac{\xi_m(\lambda)\mu_{m-1}(\lambda)}{\sqrt{\mu_{m-1}(\lambda)^2 + \xi_m(\lambda)^2}},$$

with $\mu_0(\lambda) = \|v\|$ and, referring to (2.3),

$$\xi_m(\lambda) = \left|\det((\lambda+\delta)^{-1}I - H_m)^{-1} \prod_{j=1}^{m} h_{j+1,j}\right|.$$

Accordingly, by (8.1) (see Lemma 8.1 in Appendix) we get

$$\|D(\lambda)v\| \leq \|D(\lambda)\| \, \mu_m(\lambda),$$

and we derive the a posteriori bound

$$\|y - \overline{y}\| \leq \int_\Gamma |\psi(\lambda)| \, \|D(\lambda)\| \, \mu_m(\lambda) d\lambda.$$

One can also make use of the inequality

$$\mu_m(\lambda) \leq \mu_{m,j}(\lambda) := \frac{\xi_m(\lambda)\mu_j(\lambda)}{\sqrt{\mu_j(\lambda)^2 + \xi_m(\lambda)^2}}, \tag{5.5}$$

for any $j \leq m-1$. Having at disposal the eigenvalues of of $H_{m,}$, say ϑ_j, for $j = 1,,,.m$, recalling that $h_{j+1,j} \geq 0$ we can compute $\xi_m(\lambda)$ by

$$\xi_m(\lambda) = \frac{|\lambda+\delta|^m \prod_{j=1}^m h_{j+1,j}}{\prod_{j=1}^m |1-(\lambda+\delta)\vartheta_j|}.$$

Dealing with formulas (3.5), using (5.2) and (5.5), from (5.3) we get the error bound

$$\|y - \overline{y}\| \leq \int_0^\infty \frac{|g(\lambda)|}{a+\lambda} \mu_{m,0}(-\lambda) d\lambda. \tag{5.6}$$

On the other side, working with (3.8) and taking $\vartheta = \pi/4$, that is, $\lambda = re^{\pm i\pi/4}$, by (5.2) we have

$$\begin{aligned} \|D(\lambda)\| &\leq \frac{2}{\sqrt{\left(\frac{a}{\sqrt{2}}\right)^2 + \left(r - \frac{a}{\sqrt{2}}\right)^2}} \\ &= \frac{2\sqrt{2}}{\sqrt{a^2 + \left(\sqrt{2}r - a\right)^2}}, \end{aligned}$$

and therefore from (5.4) we have

$$\|y - \overline{y}\| \leq \frac{\sqrt{2}}{\pi} \int_0^\infty \frac{\left|f\left(re^{i\frac{\pi}{4}}\right)\right| + \left|f\left(re^{-i\frac{\pi}{4}}\right)\right|}{\sqrt{a^2 + \left(\sqrt{2}r - a\right)^2}} \mu_{m,0}\left(re^{i\frac{\pi}{4}}\right) dr. \tag{5.7}$$

6 Numerical experiments

In this section we present the results of some numerical experiments. At first we take $-A$ obtained by central-differences discretization of the standard Laplacian operator with homogeneous Dirichlet boundary conditions in one and two dimensions. In one dimension the spatial domain is the interval $[0,1]$, discretized with $N = 1600$ equally spaced internal grid points, and the starting vector of the Krylov process is the pointwise discretization of $x(1-x)$. In two dimensions we consider a uniform discretization of the square $[0,1] \times [0,1]$ with $N = 2500$ internal grid points. The starting vector is the discretization of $xy(1-x)(1-y)$. In Figures 1 and 2 we consider the computation of $y = (I + tA^{\frac{\alpha}{2}})^{-1}v$, for different values of α, by using the SIKM with $\delta = t^{-2/\alpha}$ and $\delta = \sqrt{ab}$ ($a = \lambda_{\min}$, $b = \lambda_{\max}$) and comparing it with the SKM. In Figures 3 and 4 we show the same comparisons for the computation of $y = \exp(-tA^{\frac{\alpha}{2}})v$.

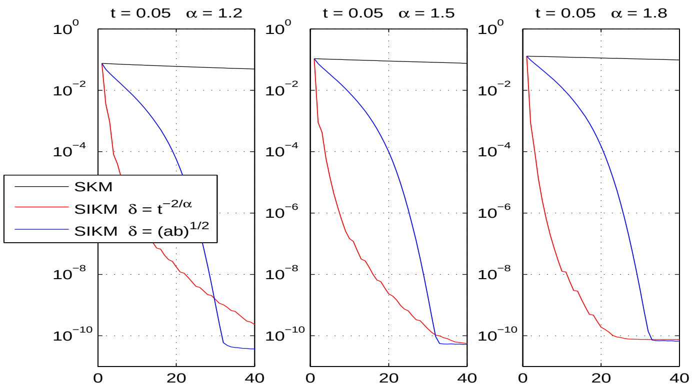

Figure 1: Convergence history for the computation of $(I + tA^{\frac{\alpha}{2}})^{-1}v$, one dimension, $N = 1600$.

Observe that for the two different values of δ considered, the shape of the error curve are different. Both give a sufficiently fast convergence, even if the value $\delta = t^{-\frac{\alpha}{2}}$ seems in general to work better. This was also confirmed by other experiments we made with other values of t.

Figure 5 refers to the two dimensional case. Therein we report the a priori bound (3.14) together with the a posteriori bounds (5.6) and (5.7), with $\delta = t^{-2/\alpha}$, again for the matrix functions considered above. We remark that all the integrals involved in the bounds are numerically evaluated by means of a composite Gauss-Legendre rule after suitable substitutions. The constant C in (3.14) has been set equal to 4 (see Remark 3.6).

As expected, the a priori bounds are pessimistic. Nevertheless, we point out that the a posteriori ones are fairly accurate.

Figures 6 and 7 concern the a priori bound (3.12), again with $C = 4$, on artificial examples. In order to simulate the spectral properties of self-adjoint

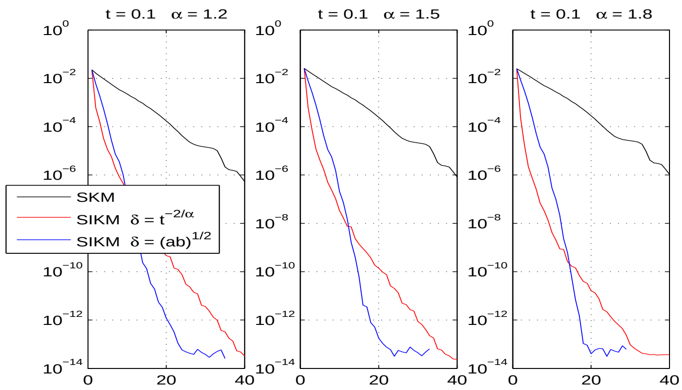

Figure 2: Convergence history for the computation of $(I+tA^{\frac{\alpha}{2}})^{-1}v$, two dimensions, $N=2500$.

unbounded operators, we consider diagonal matrices whose spectrum grows quadratically with the dimension. Our aim is to show the sublinear convergence whenever $\lambda_{\max} \to \infty$, and that this convergence rate is well captured by the a priori bound (3.12). This is particularly clear in Figure 6, where we consider the computation of $(I+tA^{\frac{\alpha}{2}})^{-1}v$ where

$$A = diag\left(k^2\right), \quad k=1,...,N, \tag{6.1}$$

and $v=(1,...,1)^T$.

In Figure 7 we consider the computation of $\exp(-tA^{\frac{\alpha}{2}})v$ with

$$A = \begin{pmatrix} diag\,(j) & \\ & diag\left(k^2\right) \end{pmatrix}, \quad j=1,...,N/2, \quad k=N/2+1,...,N, \tag{6.2}$$

and $v=(1,...,1)^T$. In this situation, the sublinear behavior is less evident because of the nature of the underlying function, that is, because the error rapidly goes to 0. Nevertheless also in this case the a priori bound is able to describe rather well the rate of convergence for large values of N.

7 Conclusion

We have analyzed the convergence of the shift-and-invert Krylov subspace method for functions of fractional powers of some differential operators. A priori error bounds have been provided. Such bounds point out a possible sublinear convergence of the method. Anyhow, they are independent of the size of the spectrum of the involved operators. This implies that, dealing with discrertizations, the rate of convergence cannot become arbitrarily slow as such discretizations are refined. A posteriori bounds were also proposed to control the behavior of the procedure.

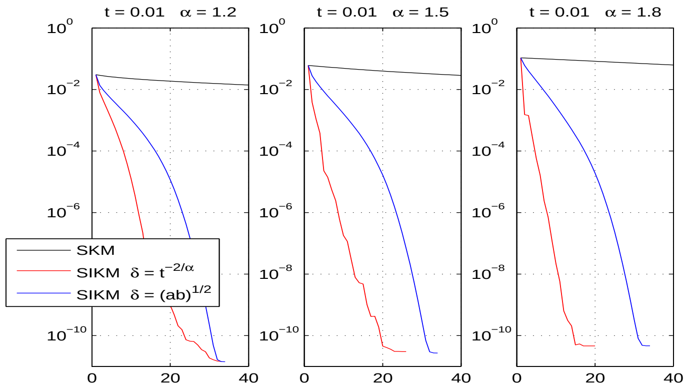

Figure 3: Convergence history for the computation of $\exp(-tA^{\frac{\alpha}{2}})v$, one dimension, $N = 1600$.

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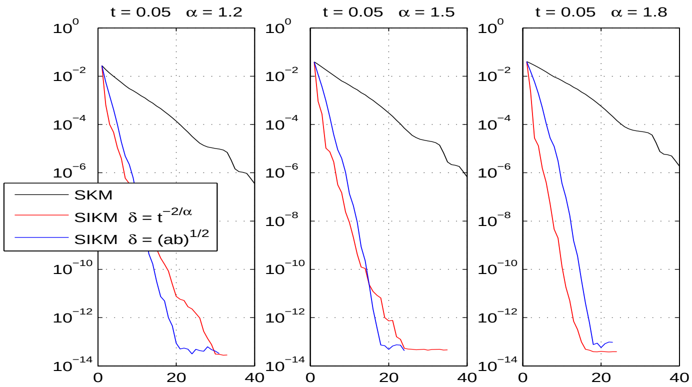

Figure 4: Convergence history for the computation of $\exp(-tA^{\frac{\alpha}{2}})v$, two dimensions, $N = 2500$.

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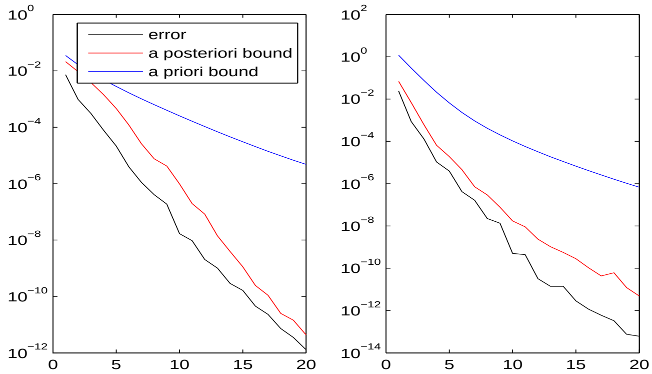

Figure 5: Two dimensional problem. Left: true error, a posteriori bound (5.6) and a priori bound (3.14) for the computation of $(I + tA^{\frac{\alpha}{2}})^{-1}v$, with $\alpha = 1.4$ and $t = 0.01$. Right: true error, a posteriori bound (5.7) and a priori bound (3.14) for $\exp(-tA^{\frac{\alpha}{2}})v$, with $\alpha = 1.6$ and $t = 0.05$. In both cases (3.14) has been used with $R = 10^5$.

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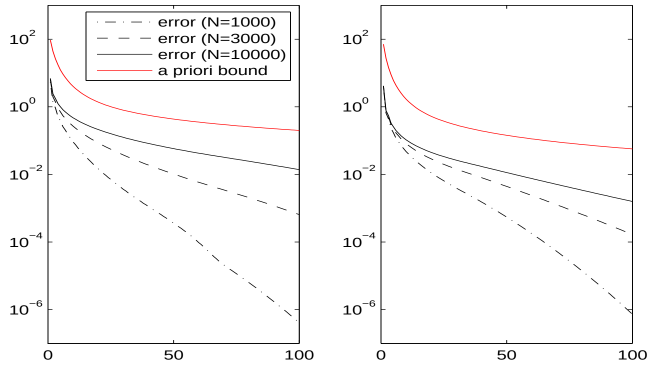

Figure 6: Error and a priori bound (3.12) for the computation of $(I+tA^{\frac{\alpha}{2}})^{-1}v$, $t = 0.01$, with A defined by (6.1) and different values of N. On the left $\alpha = 1.2$, $p = 1.8$, on the right $\alpha = 1.5$, $p = 1.5$. In both cases (3.12) has been used with $R = 10^4$.

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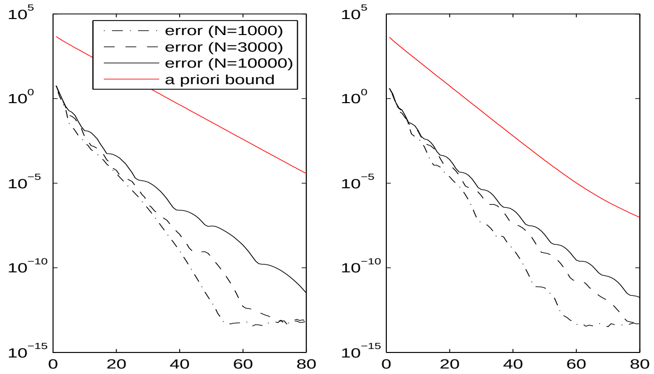

Figure 7: Error and a priori bound (3.12) for the computation of $\exp(-tA^{\frac{\alpha}{2}})v$, $t = 0.05$, with A defined by (6.2) and different values of N. On the left $\alpha = 1.4$, $p = 1.5$, on the right $\alpha = 1.7$, $p = 1.2$. In both cases (3.12) has been used with $R = 10^4$.

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8 Appendix

Lemma 8.1 *Referring to formulae (5.1), (3.1) and (3.9). Let* $v \in \mathbb{X}$, $m \geq 1, \mathcal{K}_{m+1} = \mathcal{K}_{m+1}(Z, v)$, $B_{m+1} = H_{m+1}^{-1} - \delta I$. *Then for every* $p_m \in \Pi_m$ *we have*

$$D(\lambda)v = \frac{D(\lambda)p_m(Z)v}{p_m((\lambda+\delta)^{-1})}. \tag{8.1}$$

Let $v \in \mathbb{D}(A)$, $m \geq 1, \mathcal{K}_{m+1} = \mathcal{K}_{m+1}(Z, v)$, $B_{m+1} = V_{m+1}^* A V_{m+1}$, *then (8.1) holds and*

$$D(\lambda)v = \frac{D(\lambda)p_m(Z)(A - aI)v}{(\lambda - a)p_m((\delta+\lambda)^{-1})}. \tag{8.2}$$

Moreover

$$\min_{p_m \in \Pi_m} \max_{z \in (0, \frac{1}{\delta+a}).} \left| \frac{p_m(z)}{p_m((\delta+\lambda)^{-1})} \right| \leq 2\Phi(\omega(\lambda))^{-m}. \tag{8.3}$$

Proof 8.2 *Using the identities* $(\lambda I - A) = (\lambda+\delta)I - Z^{-1}$ *and* $\lambda I - B_{m+1} = (\lambda+\delta)I - H_{m+1}^{-1}$ *we realize that* $D(\lambda)(\lambda I - A)Zp_{m-1}(Z)v = 0$ *for every* $p_{m-1} \in \Pi_{m-1}$. *Hence, we easily get (8.1). This follows similarly when* $v \in \mathbb{D}(A)$ *and* $B = V_{m+1}^* A V_{m+1}$. *In order to get (8.2), let* $w = p_m(Z)v$ *and observe that*

$$D(\lambda)w = \frac{1}{\lambda - a}((\lambda I - A)^{-1}(A - aI) - V_{m+1}(\lambda I - B_{m+1})^{-1}(B_{m+1} - aI)V_{m+1}^*)w.$$

Hence, assuming that $B_{m+1} = V_{m+1}^* A V_{m+1}$, *then (8.2) follows. Finally (8.3) follows from a well known result given in [12].*

Proof 8.3 *of Propositions 3.3. For the sake of clarity we consider the two cases separately. Consider at first (3.5). We have*

$$\|y - \overline{y}\| \leq I_1 + I_2, \tag{8.4}$$

where

$$\begin{aligned} I_1 &= \left\| \int_0^R g(\lambda) D(-\lambda) v d\lambda \right\|, \\ I_2 &= \left\| \int_R^\infty g(\lambda) D(-\lambda) v d\lambda \right\|. \end{aligned}$$

By (5.2), for $\lambda \geq 0$,

$$\|D(-\lambda)\| \leq 2/(a+\lambda).$$

Since $\sigma(Z) \subset (0, \frac{1}{\delta+a}]$, *by Lemma 8.1 we get*

$$\|D(-\lambda)v\| \leq \frac{4\,\|v\|\,\Phi(\omega(-\lambda))^{-m}}{a+\lambda}, \tag{8.5}$$

with

$$\omega(-\lambda) = \frac{\delta + 2a + \lambda}{|\delta - \lambda|}. \tag{8.6}$$

Thus we obtain

$$I_1 \leq 4S_m(R) \|v\| . \tag{8.7}$$

Using (8.6) for $\lambda > R$ and recalling that for $x \geq 0$

$$\Phi(1+x)^{-m} \leq C \exp(-m\sqrt{2x}), \tag{8.8}$$

we get

$$\Phi(\omega(-\lambda))^{-m} \leq C \exp\left(-2m\sqrt{\frac{\delta+a}{\lambda-\delta}}\right).$$

Then, by (8.5) we obtain

$$I_2 \leq C \|v\| \int_R^\infty \frac{|g(\lambda)|}{a+\lambda} \exp\left(-2m\sqrt{\frac{\delta+a}{\lambda-\delta}}\right) d\lambda.$$

Taking into account of (3.10), by Hölder inequality we get, for $q = \frac{p}{p-1}$,

$$\begin{aligned} I_2 &\leq C \|v\| s_p(R) \left(\int_R^\infty \frac{1}{\lambda^q} \exp\left(-2qm\sqrt{\frac{\delta+a}{\lambda}}\right) d\lambda\right)^{\frac{1}{q}} \\ &= C \|v\| \frac{s_p(R)}{R^{\frac{1}{p}}} \left(\int_1^\infty \frac{1}{\xi^q} \exp\left(-2qm\sqrt{\frac{\delta+a}{\xi R}}\right) d\xi\right)^{\frac{1}{q}} \\ &\leq C \|v\| \frac{2s_p(R)}{R^{\frac{1}{p}}} \left(\int_0^1 x^{2q-3} \exp\left(-2qmx\sqrt{\frac{\delta+a}{R}}\right) dx\right)^{\frac{1}{q}}. \end{aligned}$$

Observing that, for $\tau > 0$ it is

$$\begin{aligned} \int_0^1 x^{2q-3} \exp(-\tau x) dx &\leq \tau^{-2(q-1)} \int_0^\tau t^{2q-3} \exp(-t) dt && (8.9) \\ &\leq \Gamma(2(q-1))\tau^{-2(q-1)}, && (8.10) \end{aligned}$$

we obtain

$$I_2 \leq C \|v\| K_m(R).$$

Collecting this with (8.7) one proves the result.

Considering now (3.8) with $\Gamma = i\mathbb{R}$, we realize that

$$\|y - \overline{y}\| \leq \frac{1}{2\pi} \int_{-\infty}^\infty \|f(i\lambda)D(i\lambda)v\| d\lambda,$$

and therefore

$$\|y - \overline{y}\| \leq \frac{1}{2\pi}(I_1 + I_2), \tag{8.11}$$

where

$$\begin{aligned} I_1 &= \int_0^R (\|f(ir)D(ir))v\| + \|f(-ir)D(-ir)v\|)dr, \\ I_2 &= \int_R^\infty (\|f(ir)D(ir))v\| + \|f(-ir)D(-ir)v\|)dr. \end{aligned}$$

By (5.2) we clearly have

$$\|D(\pm ir)\| \le \frac{1}{\sqrt{a^2+r^2}}.$$

Therefore, by Lemma 8.1 we now obtain

$$\|D(\pm ir)v\| \le \frac{4\,\|v\|\,\Phi(\omega(\pm ir))^m}{\sqrt{a^2+r^2}}, \tag{8.12}$$

where

$$\omega(\pm ir) = \frac{\delta + a + |a \mp ir|}{|\delta \pm ir|}.$$

Then $I_1 \le 4S_m(R)\,\|v\|$. *Moreover, one verifies that for* $r \ge R$ *it is*

$$\omega(\pm ir)) \ge 1 + \frac{\delta+a}{3r}.$$

Therefore, by (8.8) we have

$$\Phi(\omega(\pm ir))^{-m} \le C\exp\left(-m\sqrt{\frac{2(\delta+a)}{3r}}\right). \tag{8.13}$$

Finally, by assumption (3.11), by (8.12) and (8.13) we obtain, for $q = \frac{p}{p-1}$,

$$I_2 \le C\,\|v\|\,s_p(R)\left(\int_R^\infty r^q \exp\left(-qm\sqrt{\frac{\delta+a}{2r}}\right)dr\right)^{\frac{1}{q}},$$

and, arguing as before, we finally have

$$I_2 \le C\,\|v\|\,K_m(R). \tag{8.14}$$

This concludes the proof.

Proof 8.4 *of Proposition 3.4. The statement can be proved arguing as before using now (8.2).*

Proof 8.5 *of Proposition 3.5. The proof follows from (8.4) and (8.11) using again (8.2).*