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Analysis of BURA and BURA-based approximations of fractional powers of sparse SPD matrices

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Abstract Numerical methods applicable to the approximation of spectral fractional diffusion operators in multidimensional domains with general geometry are analyzed. Over the past decade, several approaches have been proposed to approximate the inverse operator $\mathcal{A}^{-\alpha}$, $\alpha \in (0,1)$. Despite their different origins, they can all be written as a rational approximation. Let the matrix $\mathbb{A}$ be obtained after finite difference or finite element discretization of $\mathcal{A}$. The BURA (Best Uniform Rational Approximation) method was introduced to approximate the inverse matrix $\mathbb{A}^{-\alpha}$ based on an approximation of the scallar function z^{α}, $\alpha \in (0,1)$, $z \in [0,1]$.

In this paper we study BURA and BURA-based methods for fractional powers of sparse symmetric and positive definite (SPD) matrices, presentiing the concept, general framework and error analysis. Our contributions concern approximations of $\mathbb{A}^{-\alpha}$ and $\mathbb{A}^{\alpha}$ for arbitrary $\alpha > 0$, thus significantly expanding the range of available currently results. Assymptotically accurate error estimates are obtained. The rate of convergence is exponential with respect to the degree of BURA. Numerical results are presented to illustrate and better interpret the theoretical estimates.

Keywords fractional elliptic operators · BURA method · error estimates · computational complexity

Mathematics Subject Classification (2010) 65F08 · 65N30 · 65N22

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1 Introduction

Let us consider the second order self-adjoint elliptic equation

$$\begin{aligned} -\nabla \cdot (a(x)\nabla v(x)) &= g(x), \qquad \text{for } x \in \Omega, \\ v(x) &= 0, \qquad \text{for } x \in \partial\Omega, \end{aligned} \tag{1.1}$$

where Ω is a bounded domain in $\mathbb{R}^d$, $d \geq 1$, assuming that $0 < a_0 \leq a(x)$, a_0 is a constant. With the problem (1.1) we associate the self-adjoint positive definite operator $\mathcal{A}$ defined in terms of the weak form of (1.1), namely, $v(x)$ is the unique function in $V = H_0^1(\Omega)$ satisfying

$$\int_\Omega \Big(a(x)\nabla v(x) \cdot \nabla \theta(x) \Big)\, dx = \int_\Omega g(x)\theta(x)\, dx \qquad \text{for all } \theta \in V. \tag{1.2}$$

For $g \in L^2(\Omega)$, (1.2) can be written in the form

$$\mathcal{A}v = g. \tag{1.3}$$

Let us consider now the the fractional diffusion equation

$$\mathcal{A}^\alpha u = f, \tag{1.4}$$

where $f \in L^2(\Omega)$ and $\alpha > 0$. We follow the spectral definition of $\mathcal{A}^\alpha$ which can be written in the form

$$\mathcal{A}^\alpha u = \sum_{i=1}^{\infty} \lambda_i^\alpha (u, \phi_i)\phi_i \;\; \text{so that } u = \sum_{i=1}^{\infty} \lambda_i^{-\alpha} (f, \phi_i)\phi_i. \tag{1.5}$$

Here $\lambda_i \in (0, \infty)$ and ϕ_i are the eigenvalues and eigenfunctions of $\mathcal{A}$, and $(\cdot, \cdot)$ is the inner product in $L^2(\Omega)$. It is important to note that $\lambda_1 > \underline{\lambda} > 0$ is uniformly bounded from below. Such a bound can be obtained using the coercivity of the biliner form in (1.2) and the Poincaré-Friedrichs inequality [32]. A problem-oriented discussion on the spectral properties of $\mathcal{A}$ in the context of the BURA method can be found in [20].

The inverse of the spectral fractional operator $\mathcal{A}^{-\alpha}$ can be equivalently defined by Dunford-Taylor integral, which in turn can be transformed, when $\alpha \in (0, 1)$, into the Balakrishnan integral, e.g. [3],

$$u = \mathcal{A}^{-\alpha} f = \frac{\sin(\pi\alpha)}{\pi} \int_0^\infty \nu^{-\alpha} (\nu\mathcal{I} + \mathcal{A})^{-1} f\, d\nu. \tag{1.6}$$

The following fractional order linear system is a discrete form of (1.5):

$$\mathbb{A}^\alpha \mathbf{u} = \mathbf{f}, \quad \text{or equivalently} \quad \mathbf{u} = \mathbb{A}^{-\alpha}\mathbf{f}. \tag{1.7}$$

For simplicity of presentation, we will assume in what follows that $\mathbb{A} \in \mathbb{R}^{N\times N}$ is a sparse symmetric and positive definite (SPD) matrix. This is, for example, valid in the case of a finite-difference approximation on a uniform grid of the differential operator in (1.1). Then $\mathbf{u} \in \mathbb{R}^N$ approximates u at the interior N

grid points, and $\mathbf{f} \in \mathbb{R}^N$ denotes the vector of the values of f at the same grid points. Similarly to (1.3), the spectral decomposition of $\mathbb{A}$ is used to define $\mathbb{A}^\alpha$, thus obtaining the equalities:

$$\mathbb{A}^\alpha \mathbf{u} = \sum_{i=1}^{N} \mu_i^\alpha (\mathbf{f}, \Psi_i)\Psi_i \quad \text{so that } \mathbf{u} = \sum_{i=1}^{N} \mu_i^{-\alpha} (\mathbf{f}, \Psi_i)\Psi_i. \tag{1.8}$$

Here $\mu_i > 0$ and Ψ_j are the eigenvalues and eigenvectors of $\mathbb{A}$, and $(\cdot, \cdot)$ is the Euclidean inner product. We can show that as an approximation of λ_1, $\mu_1 > 0$ is also uniformly bounded from below.

Remark 1 If the finite element discretization is applied to (1.2), the matrix $\mathbb{A}$ in (1.7) is expressed by the stiffness matrix $\mathbb{K}$ and the mass matrix $\mathbb{M}$ in the form $\mathbb{A} = \mathbb{M}^{-1}\mathbb{K}$. The mass and stiffness matrices are sparse and SPD, and $\mathbb{A}$ is also SPD with respect to the energy inner product associated with $\mathbb{M}$. This allows the general framework of SPD matrix methods to be applied, preserving computational efficiency when dealing only with sparse matrices (see e.g. [19, 20]).

The fractional diffusion equation (1.4) is non-local. In the discrete case, the matrix $\mathbb{A}^\alpha$ in (1.7) is SPD but dense. Except for some simplified cases, we are unable to compute the eigenvalues and eigenfunctions/eigenvectors of $\mathbb{A}$. Therefore, the formulas (1.5) and (1.8) are not applicable to the numerical solution of the problem.

The ideas in the work of Caffarelli and Silvestre [11] are among the strongest drivers in the later development over past decade of numerical methods for spectral fractional in space diffusion problems. They have proved that the fractional Laplacian for $\alpha \in (0, 1)$ can be obtained from the harmonic extension problem to the upper half space as the operator that maps the Dirichlet boundary condition to the Neumann condition. As a result, the solution of fractional Laplacian problem is obtained from the relation $u(x) = U(x, 0)$ where $U : \Omega \times \mathbb{R}_+ \to \mathbb{R}$ is a solution of the equation

$$-\operatorname{div}\left(y^{1-2\alpha}\nabla U(x, y)\right) = 0, \quad (x, y) \in \{\Omega \times \mathbb{R}_+\}.$$

Here $U(\cdot, y)$ satisfies the boundary conditions in (1.1) and in addition

$$\lim_{y\to\infty} U(x, y) = 0 \quad \text{as well as} \quad \lim_{y\to 0^+} \left(-y^{1-2\alpha} U_y(x, y)\right) = f(x), \quad x \in \Omega.$$

Although very different in their origin, there is a number of approaches that can be seen as transformation of the d-dimensional non-local fractional Laplacian with $\alpha \in (0, 1)$ to a $(d + 1)$-dimensional standard (local) equation. Without seeking completeness of the list, among them are:

A1. Extension from $\Omega \subset \mathbb{R}^d$ to an elliptic problem in $\Omega \times (0, \infty)$, see e.g. [30, 31];
A2. Reformulation as a pseudo-parabolic problem in $(x, t) \in \Omega \times (0, 1)$, see e.g. [14, 17, 35];

A3. Methods based on approximation of the Dunford-Taylor integral representation of the solution, [8,9,10];
A4. Methods based on the best uniform rational approximation (BURA) of z^α, $z \in [0,1]$, see e.g. [21,20,22].

As shown in [24], methods that implement approaches A1.-A3. can be interpreted as some rational approximation of $\mathbb{A}^\alpha$. In this sense (when applicable) BURA methods have better computational complexity in terms of the number of auxiliary sparse solutions of SPD systems involved.

A survey on numerical methods for spectral space-fractional diffusion problems is provided in [19]. Among the results in the last few years, we can note the following areas and some of the publications related to them: (i) further development of efficient numerical methods for space-fractional differential equations [1,4,12,16]; (ii) time-dependent space-fractional diffusion problems [13, 15,36]; (iii) fractional Sobolev spaces in coupled and multiphysics problems, [7,23,27]; (iv) fractional elliptic stochastic equations, [2,6,26].

Our research is motivated by the increased interest in the further development of robust and computationally efficient numerical methods for wider classes of problems that involve fractional powers of diffusion operators. We analyze approximations of $\mathbb{A}^{-\alpha}$ and $\mathbb{A}^\alpha$ for arbitrary $\alpha > 0$. Thereby we significantly expand the theory of BURA methods. Here, along with BURA, we also analyze BURA-like methods. The latter are defined as the product of a certain best uniform rational approximation and some integer power of $\mathbb{A}$. The new results substantially build on the results for the $\alpha \in (0,1)$ case, which has been intensively studied over the last decade.

The contribution of this paper can be divided into two parts. The part related to solving the system $\mathbb{A}^\alpha \mathbf{u} = \mathbf{f}$ contains both comprehensive theoretical and experimental results. The main point here is the conclusion that the BURA method is preferable and more efficient than the BURA-like method. In some ways, the part about evaluating $\mathbb{A}^\alpha \mathbf{f}$ is even more challenging. For this problem, theoretical error estimates have been obtained only for the BURA-like method. However, the presented numerical experiments show that the corresponding BURA method again has the advantage.

The paper is organized as follows. Basic results on best uniform rational approximation of z^α on $[0,1]$ for $\alpha > 0$ are presented in Section 2. Then, some implementation issues and computational complexity of the related BURA methods are discussed. The numerical solution of system $\mathbb{A}^\alpha \mathbf{u} = \mathbf{f}$ based on BURA approximation of $\mathbb{A}^{-\alpha}$ is analysed in Section 3. The BURA-based method for approximate matrix vector multiplication with $\mathbb{A}^\alpha$ is considered in the next section. It is worth noting that this problem is equivalent to solving fractional order linear SPD systems with a negative power. The numerical results included in the last Sections 2 - 3 build on the better understanding of the theoretical error estimates. Short concluding remarks are given at the end.

2 Best uniform rational approximation of z^α

2.1 Exponential convergence error estimate

Known basic results in the general case of $\alpha > 0$ are presented in this section. Taking the diagonal of the Walsh table we consider $\mathcal{R}_k$ to be the set of rational functions

$$\mathcal{R}_k = \big\{ r_k(z) := P_k(z)/Q_k(z),\ P_k \in \mathcal{P}_k,\ \text{and}\ \ Q_k \in \mathcal{P}_k,\ \text{monic} \big\}$$

with $\mathcal{P}_k$ set of algebraic polynomials of degree k. The best uniform rational approximation (BURA) $r_{\alpha,k}(z)$ of z^α on $[0,1]$ is then defined as

$$r_{\alpha,k}(z) := \underset{r_k(z)\in\mathcal{R}_k}{\operatorname{argmin}} \max_{z\in[0,1]} |r_k(z) - z^\alpha|. \tag{2.1}$$

The problem (2.1) has been studied extensively in the past, see e.g. [34]. Denoting the error by

$$E_{\alpha,k} := \max_{z\in[0,1]} |r_{\alpha,k}(z) - z^\alpha|, \tag{2.2}$$

it is shown that there is a constant $C_\alpha > 0$, independent of k, such that

$$E_{\alpha,k} \le C_\alpha e^{-2\pi\sqrt{k\alpha}}. \tag{2.3}$$

The asymptotic behaviour of C_α is analysed in [34], where the following estimate is proven in Theorem 1:

$$\lim_{k\to\infty} e^{2\pi\sqrt{\alpha k}} E_{\alpha,k} = 4^{1+\alpha} |\sin \pi\alpha|$$

and therefore

$$\lim_{k\to\infty} E_{\alpha,k} = e^{-2\pi\sqrt{\alpha k}} 4^{1+\alpha} |\sin \pi\alpha|. \tag{2.4}$$

Remark 2 The limes (2.4) gives a sharp asymptotic approximation of $E_{\alpha,k}$. So, for example, for $\alpha = 1.5$ and sufficiently large k we get

$$E_{1.5,k} \approx 32 e^{-\pi\sqrt{6k}}.$$

2.2 Implementation issues

The min-max problem (2.1) is highly nonlinear. In [22], the Remez algorithm is used to find the best uniform rational approximation of z^α. Due to exponential clustering of the poles and zeros of $r_{\alpha,k}$ around zero the algorithm is sensitive to the precision of the computer arithmetic. For example, in [37] results for six values of $\alpha \in (0,1)$ are reported for degree $k \le 30$ by using computer arithmetic with 200 significant digits. So, although doable, the Remez algorithm was considered as a challenge to a wider application of BURA method for higher degrees k.

This difficulty is avoided by AAA (Adaptive Antoulas-Anderson) method proposed in [29]. The numerical stability of AAA comes from barycentric representation of rational functions as a quotient of two partial fractions:

$$r_k(z) = \sum_{i=1}^{k} \frac{a_i}{z - t_i} \Big/ \sum_{i=1}^{k} \frac{b_i}{z - t_i}.$$

The numbers $\{t_k\}$ are not the poles of r_k, but rather a set of support points that are chosen to enable stability, even when poles are exponentially clustered. Further improvement of convergence is proposed in [25] and its software implementation BRASIL [33] which is used in the numerical tests in next two sections.

Let us consider the BURA method introduced in [20]. The BURA approximation of the solution of (1.8) is defined as

$$\mathbf{u} \approx \mu_1^{-\alpha} r_{\alpha,k}(\mu_1 \mathbb{A}^{-1})\mathbf{f}. \tag{2.5}$$

The roots ζ_i and poles d_i of $r_{\alpha,k}(z)$ satisfy the interlacing inequalities [22,34]

$$0 > \zeta_1 > d_1 > \zeta_2 > d_2 > \cdots > \zeta_k > d_k. \tag{2.6}$$

Then $r_{\alpha,k}(z)$ can be represented as a sum of partial fractions. This allows to write the BURA approximation of $\mathbb{A}^{-\alpha}$ in the form

$$\mathbb{A}^{-\alpha} \approx \tilde{c}_0 \mathbb{I} + \sum_{i=1}^{k} \tilde{c}_i (\mathbb{A} - \tilde{d}_i \mathbb{I})^{-1}, \tag{2.7}$$

where $\tilde{c}_i \geq 0$ and $\tilde{d}_i < 0$. Thus, the BURA method reduces solving the dense linear system (1.8) (the non-local fractional diffusion problem) to solving k systems with sparse SPD matrices $\mathbb{A} - \tilde{d}_i \mathbb{I}$.

The exponential convergence rate (2.3-2.4) and the representation of the algorithm in the form (2.7) characterize the computational efficiency of the BURA methods. The basic properties and performance issues presented above are studied in detail in the case of $\alpha \in (0, 1)$ in [20], see also [19,22]. The aim of the research in the next two sections is to extend the constructions and analysis of BURA-based methods for arbitrary positive fractional (excluding integers) degree α, that is for $\alpha \in \mathbb{R}^+ \setminus \mathbb{Z}$.

3 Solution of linear systems: approximation of $\mathbb{A}^{-\alpha}$

In this section we analyze methods for numerical solution of the system

$$\mathbb{A}^{\alpha}\mathbf{u} = \mathbf{f}, \qquad \alpha \in \mathbb{R}^+ \setminus \mathbb{Z}. \tag{3.1}$$

Two variants of exponentially convergent methods that use BURA approximation of the inverse of fractional power of symmetric SPD matrix are analysed.

3.1 BURA method

Following (2.5) we consider the BURA approximation $\mathbf{w}$ in the form

$$\mathbf{w} := \mu_1^{-\alpha} r_{\alpha,k}(\mu_1 \mathbb{A}^{-1})\mathbf{f}.$$

The analysis in [20] (see also [19] and the references therein) is for $\alpha \in (0,1)$. In the following theorem, we extend the study to $\alpha \in \mathbb{R}^+ \setminus \mathbb{Z}$.

Theorem 1 *For each $\alpha \in \mathbb{R}^+ \setminus \mathbb{Z}$, the BURA approximation $\mathbf{w}$ of the solution of (3.1) $\mathbf{u}$ satisfies the exponential error estimate*

$$||\mathbf{u} - \mathbf{w}||_{\ell_2} \leq C_\alpha \mu_1^{-\alpha} e^{-2\pi\sqrt{k\alpha}} ||\mathbf{f}||_{\ell_2}. \tag{3.2}$$

Proof We follow the approach suggested in [22]. Let us write $\mathbf{u}$ in the form

$$\mathbf{u} = \mu_1^{-\alpha}(\mu_1 \mathbb{A}^{-1})^\alpha \mathbf{f}.$$

Utilizing the orthonormal basis of eigenvectors of $\mathbb{A}$ we get the representations

$$\mathbf{f} = \sum_{i=1}^{n} (\Psi_i, \mathbf{f})\Psi_i,$$

$$\mathbf{u} = \mu_1^{-\alpha} \sum_{i=1}^{n} \left(\frac{\mu_1}{\mu_i}\right)^\alpha (\Psi_i, \mathbf{f})\Psi_i = \mu_1^{-\alpha} \sum_{i=1}^{n} \nu_i^\alpha (\Psi_i, \mathbf{f})\Psi_i,$$

$$\mathbf{w} = \mu_1^{-\alpha} \sum_{i=1}^{n} r_{\alpha,k}\left(\frac{\mu_1}{\mu_i}\right) (\Psi_i, \mathbf{f})\Psi_i = \mu_1^{-\alpha} \sum_{i=1}^{n} r_{\alpha,k}(\nu_i)(\Psi_i, \mathbf{f})\Psi_i,$$

where $\nu_i := \mu_1/\mu_i \in (0,1]$. Then

$$||\mathbf{u} - \mathbf{w}||_{\ell_2}^2 = \mu_1^{-2\alpha} \sum_{i=1}^{n} \left(\nu_i^\alpha - r_{\alpha,k}(\nu_i)\right)^2 (\Psi_i, \mathbf{f})^2$$

$$\leq \mu_1^{-2\alpha} \max_{\nu_i} |\nu_i^\alpha - r_{\alpha,k}(\nu_i)|^2 \sum_{i=1}^{n} (\Psi_i, \mathbf{f})^2.$$

Now, applying (2.4), we conclude that

$$||\mathbf{u} - \mathbf{w}||_{\ell_2} \leq \mu_1^{-\alpha} E_{\alpha,k} ||\mathbf{f}||_{\ell_2} \leq C_\alpha \mu_1^{-\alpha} e^{-2\pi\sqrt{k\alpha}} ||\mathbf{f}||_{\ell_2},$$

thereby competing the proof. □

Corollary 1 *For every arbitrary small $\epsilon > 0$, there exits integer k such that*

$$||\mathbf{u} - \mathbf{w}||_{\ell_2} \leq (1+\epsilon)\mu_1^{-\alpha} e^{-2\pi\sqrt{k\alpha}} 4^{1+\alpha} |\sin \pi\alpha| \; ||\mathbf{f}||_{\ell_2}. \tag{3.3}$$

This asymptotic estimate follows directly from (3.2), where (2.4) is applied to C_α.

3.2 BURA-based method

In this section, we consider an alternative approach reducing the problem to the currently well-studied case of fractional order in $(0,1)$. We write $\alpha \in \mathbb{R}^+ \backslash \mathbb{Z}$ in the form

$$\alpha = \lfloor \alpha \rfloor + \beta := m + \beta, \qquad m := \lfloor \alpha \rfloor \in \mathbb{Z}, \qquad \beta \in (0,1).$$

Then, $\mathbb{A}^\alpha = \mathbb{A}^m \mathbb{A}^\beta$ and

$$\mathbf{u} = \mathbb{A}^{-m}\mathbb{A}^{-\beta}\mathbf{f} = \mu_1^{-m-\beta} \sum_{i=1}^{n} \nu_i^{m+\beta} (\Psi_i, \mathbf{f}) \Psi_i,$$

where following the notations from previous section, $\nu_i = \mu_1/\mu_i \in (0,1]$. Here, we analyze the BURA-based approximation $\underline{\mathbf{w}}$

$$\underline{\mathbf{w}} := \mathbb{A}^{-m} \mu_1^{-\beta} r_{\beta,k}(\mu_1 \mathbb{A}^{-1}) \mathbf{f}. \tag{3.4}$$

Theorem 2 *For each $\alpha \in \mathbb{R}^+ \backslash \mathbb{Z}$, the introduced in* (3.4) *BURA-based approximation $\underline{\mathbf{w}}$ of the solution* $\mathbf{u}$ *of* (3.1) *satisfies the exponential error estimate*

$$||\mathbf{u} - \underline{\mathbf{w}}||_{\ell_2} \leq C_{(\alpha - \lfloor \alpha \rfloor)} \mu_1^{-\alpha} e^{-2\pi\sqrt{k(\alpha - \lfloor \alpha \rfloor)}} ||\mathbf{f}||_{\ell_2}. \tag{3.5}$$

Proof In contrast to the representation in the proof of Theorem 1, the BURA-based approximation is presented in the form

$$\begin{aligned} \underline{\mathbf{w}} &:= \mu_1^{-m-\beta} \sum_{i=1}^{n} \left(\frac{\mu_i}{\mu_1} \right)^{-m} r_{\beta,k} \left(\frac{\mu_1}{\mu_i} \right) (\Psi_i, \mathbf{f}) \Psi_i \\ &= \mu_1^{-m-\beta} \sum_{i=1}^{n} \nu_i^m r_{\beta,k}(\nu_i) (\Psi_i, \mathbf{f}) \Psi_i. \end{aligned}$$

Now, $\nu_i^m \in (0,1]$ is used to get the estimates

$$\begin{aligned} ||\mathbf{u} - \underline{\mathbf{w}}||_{\ell_2}^2 &= \left(\mu_1^{-m-\beta} \right)^2 \sum_{i=1}^{n} \left[\nu_i^{m+\beta} - \nu_i^m r_{\beta,k}(\nu_i) \right]^2 (\Psi_i, \mathbf{f})^2 \\ &\leq \left(\mu_1^{-m-\beta} \right)^2 \max_{\nu_i} \left[\nu_i^m \left(\nu_i^\beta - r_{\beta,k}(\nu_i) \right) \right]^2 \sum_{i=1}^{n} (\Psi_i, \mathbf{f})^2 \\ &\leq \left(\mu_1^{-m-\beta} \right)^2 E_{\beta,k}^2 ||\mathbf{f}||_{\ell_2}^2. \end{aligned}$$

Finally

$$||\mathbf{u} - \underline{\mathbf{w}}||_{\ell_2} \leq C_{(\alpha - m)} \mu_1^{-\alpha} e^{-2\pi\sqrt{k(\alpha - m)}} ||\mathbf{f}||_{\ell_2}, \tag{3.6}$$

which completes the proof. □

Corollary 2 *For every arbitrary small $\epsilon > 0$, there exits integer k such that*

$$||\mathbf{u} - \underline{\mathbf{w}}||_{\ell_2} \leq (1+\epsilon) \mu_1^{-\alpha} e^{-2\pi\sqrt{k(\alpha - \lfloor \alpha \rfloor)}} 4^{1+(\alpha - \lfloor \alpha \rfloor)} |\sin \pi(\alpha - \lfloor \alpha \rfloor)| \; ||\mathbf{f}||_{\ell_2}. \tag{3.7}$$

Here, the asymptotic estimate follows from (3.5), applying (2.4) to bound $C_{(\alpha - \lfloor \alpha \rfloor)}$.

3.3 Comparative analysis

Theorem 1 and Theorem 2 as well as the corresponding asymptotic estimates (3.3) - (3.7) show a clear advantage of BURA compared to the BURA-based method. Now let's consider, for example, the case $\alpha = 1.5$. Without any limitations on the conclusions, we can assume for simplicity of comparison that $\mu_1 = 1$. Then, applying Corollary (3.3) and Corollary (3.7), we obtain the following estimates for the asymptotic (i.e., for sufficiently large k) behavior of the relative errors:

– BURA method:

$$\frac{||\mathbf{u} - \mathbf{w}||_{\ell_2}}{||\mathbf{f}||_{\ell_2}} \approx 32e^{-\pi\sqrt{6k}}; \tag{3.8}$$

– BURA-based method:

$$\frac{||\mathbf{u} - \underline{\mathbf{w}}||_{\ell_2}}{||\mathbf{f}||_{\ell_2}} \approx 8e^{-\pi\sqrt{2k}}. \tag{3.9}$$

As can be seen, for this particular example the estimates are quite close.

3.4 Best uniform rational approximation of $z^{-\alpha}$, $z \in [1, \bar{\kappa}]$ and BRASIL based experimental study.

We assume in this section that $\bar{\kappa} \geq \kappa(\mathbb{A})$ and consider the best uniform rational approximation $\hat{r}_{\alpha,k,\bar{\kappa}}$ of $z^{-\alpha}$, $z \in [1, \bar{\kappa}]$ defined as

$$\hat{r}_{\alpha,k,\bar{\kappa}}(z) := \underset{r_k(z)\in\mathcal{R}_k}{\operatorname{argmin}} \max_{z\in[1,\bar{\kappa}]} |r_k(z) - z^{-\alpha}|, \tag{3.10}$$

denoting the corresponding error by

$$\hat{E}_{\alpha,k,\bar{\kappa}} := \max_{z\in[1,\bar{\kappa}]} |\hat{r}_{\alpha,k,\bar{\kappa}}(z) - z^{-\alpha}|. \tag{3.11}$$

We consider the approximation $\hat{\mathbf{w}}$ of $\mathbf{u}$,

$$\hat{\mathbf{w}} := \mu_1^{-\alpha}\hat{r}_{\alpha,k,\delta}(\frac{1}{\mu_1}\mathbb{A})\mathbf{f}. \tag{3.12}$$

Lemma 1 *For each $\alpha \in \mathbb{R}^+ \setminus \mathbb{Z}$, the approximation $\hat{\mathbf{w}}$ of the solution of* (3.1) $\mathbf{u}$ *satisfies the error estimate*

$$||\mathbf{u} - \hat{\mathbf{w}}||_{\ell_2} \leq \mu_1^{-\alpha}\hat{E}_{\alpha,k,\bar{\kappa}}||\mathbf{f}||_{\ell_2}. \tag{3.13}$$

Proof Following the spectral decomposition approach from the proof of Theorem 3.2 we get the representations

$$\mathbf{f} = \sum_{i=1}^{n}(\Psi_i, \mathbf{f})\Psi_i,$$

$$\mathbf{u} = \mu_1^{-\alpha} \sum_{i=1}^{n} \left(\frac{\mu_1}{\mu_i}\right)^{\alpha} (\Psi_i, \mathbf{f})\Psi_i = \mu_1^{-\alpha} \sum_{i=1}^{n} \hat{\nu}_i^{-\alpha} (\Psi_i, \mathbf{f})\Psi_i,$$

$$\hat{\mathbf{w}} = \mu_1^{-\alpha} \sum_{i=1}^{n} \hat{r}_{\alpha,k,\bar{\kappa}} \left(\frac{\mu_i}{\mu_1}\right) (\Psi_i, \mathbf{f})\Psi_i = \mu_1^{-\alpha} \sum_{i=1}^{n} \hat{r}_{\alpha,k,\bar{\kappa}}(\hat{\nu}_i)(\Psi_i, \mathbf{f})\Psi_i,$$

where $\hat{\nu}_i := \mu_i/\mu_1 \in [1, \kappa(\mathbb{A})] \subset [1, \bar{\kappa}]$. Then

$$\begin{aligned} ||\mathbf{u} - \hat{\mathbf{w}}||_{\ell_2}^2 &= \mu_1^{-2\alpha} \sum_{i=1}^{n} \left(\hat{\nu}_i^{-\alpha} - \hat{r}_{\alpha,k,\bar{\kappa}}(\hat{\nu}_i)\right)^2 (\Psi_i, \mathbf{f})^2 \\ &\leq \mu_1^{-2\alpha} \max_{\hat{\nu}_i} |\hat{\nu}_i^{-\alpha} - \hat{r}_{\alpha,k,\bar{\kappa}}(\hat{\nu}_i)|^2 \sum_{i=1}^{n} (\Psi_i, \mathbf{f})^2 \\ &= \mu_1^{-2\alpha} \hat{E}_{\alpha,k,\bar{\kappa}}^2 ||\mathbf{f}||_{\ell_2}^2, \end{aligned}$$

thus completing the proof. □

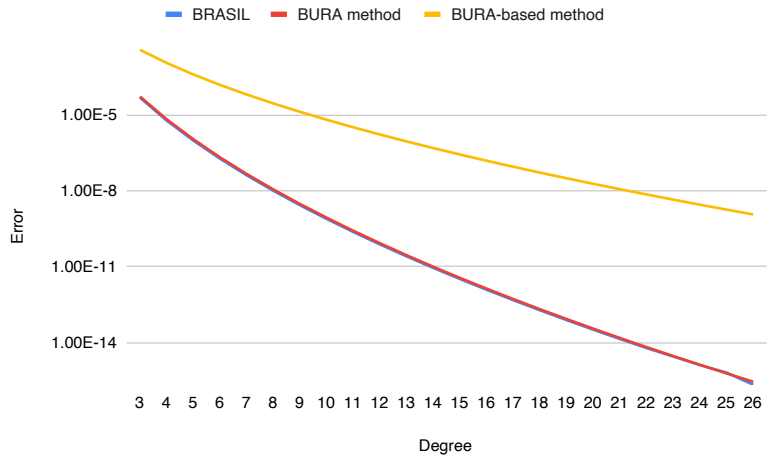

Fig. 1 Relative error of $\hat{w}$ ($\hat{r}_{\alpha,k,\bar{\kappa}}$ is computed by BRASIL with $\bar{\kappa} = 10^{12}$), and the corresponding estimates (3.8) of BURA and (3.9) of BURA-based methods versus the degree k, $\alpha = 1.5$.

The definition (3.12) more directly addresses the problem of the approximation of $\mathbb{A}^{-\alpha}\mathbf{f}$. It can also be seen that the estimate (3.13) looks quite similar to (3.2). Here, the essential difference is that we have no theoretical analysis of either the properties of the best uniform rational approximation $\hat{r}_{\alpha,k,\bar{\kappa}}$ or the estimate of $\hat{E}_{\alpha,k,\bar{\kappa}}$.

Now the software BRASIL (best rational approximation by successive interval length adjustment) [33] is used to compute $\hat{r}_{\alpha,k,\bar{\kappa}}$ and the corresponding error $\hat{E}_{\alpha,k,\bar{\kappa}}$. For direct comparison with (3.8) and (3.9), we assume that

$\mu_1 = 1$ and run test problems for $\alpha = 1.5$ and $\bar{\kappa} = 10^{12}$, varying the degree $3 \le k \le 26$. The test results of are shown in Fig. 1. We see that the relative error of $\hat{w}$ practically coincides with that of BURA calculated by (3.8), which illustrates the accuracy of Theorem 1. As expected, the advantage of BURA is pronounced compared to the BURA-based approximation, becoming stronger as k increases.

4 Matrix vector multiplication: approximation of $\mathbb{A}^{\alpha}$

Computing $\mathbf{v} = \mathbb{A}^{\alpha}\mathbf{f}$ is equivalent to solving a system with $\mathbb{A}^{-\alpha}$. At the same time, the theory of the best uniform rational approximation of z^s, $z \in [0,1]$ [34] does not include the case of negative powers s. This is the reason why we proceed directly with the construction of a BURA-based method. As will bee shown, the matrix vector multiplication with $\mathbb{A}^{\alpha}$ is computationally more expensive task than solving a system with the same matrix.

4.1 BURA-based method

Here, we write $\alpha \in \mathbb{R}^+ \setminus \mathbb{Z}$ in the form

$$\alpha = \lceil \alpha \rceil - \gamma := M - \gamma, \qquad M := \lceil \alpha \rceil \in \mathbb{Z}, \qquad \gamma \in (0,1).$$

Then, $\mathbb{A}^{\alpha} = \mathbb{A}^{M}\mathbb{A}^{-\gamma}$ and

$$\mathbf{v} = \mathbb{A}^{M}\mathbb{A}^{-\gamma}\mathbf{f} = \sum_{i=1}^{n} \mu_i^{M-\gamma}(\Psi_i, \mathbf{f})\Psi_i = \mu_1^{M-\gamma}\sum_{i=1}^{n} \nu_i^{-(M-\gamma)}(\Psi_i, \mathbf{f})\Psi_i,$$

where, as in the previous sections, $\nu_i = \mu_1/\mu_i \in (0,1]$.

Here, we analyze the following BURA-based approximation $\underline{\mathbf{v}}$ of $\mathbf{v}$:

$$\underline{\mathbf{v}} := \mathbb{A}^{M}\mu_1^{-\gamma} r_{\gamma,k}(\mu_1 \mathbb{A}^{-1})\mathbf{f}. \tag{4.1}$$

Theorem 3 *For each $\alpha \in \mathbb{R}^+ \setminus \mathbb{Z}$, the introduced in* (4.1) *BURA-based approximation $\underline{\mathbf{v}}$ of $\mathbf{v} = \mathbb{A}^{\alpha}$ satisfies the error estimate*

$$||\mathbf{u} - \underline{\mathbf{w}}||_{\ell_2} \le C_{\lceil\alpha\rceil-\alpha}\ \mu_1^{\alpha}\kappa^{\lceil\alpha\rceil}(\mathbb{A})\ e^{-2\pi\sqrt{k(\lceil\alpha\rceil-\alpha)}}||\mathbf{f}||_{\ell_2}. \tag{4.2}$$

Proof The BURA-based approximation is presented in the form

$$\underline{\mathbf{v}} := \mu_1^{M-\gamma}\sum_{i=1}^{n}\left(\frac{\mu_i}{\mu_1}\right)^{M} r_{\gamma,k}\left(\frac{\mu_1}{\mu_i}\right)(\Psi_i, \mathbf{f})\Psi_i$$

$$= \mu_1^{M-\gamma}\sum_{i=1}^{n}\nu_i^{-M} r_{\gamma,k}(\nu_i)(\Psi_i, \mathbf{f})\Psi_i.$$

Now,

$$||\mathbf{v}-\underline{\mathbf{v}}||^2_{\ell_2} = \left(\mu_1^{M-\gamma}\right)^2 \sum_{i=1}^{n} \left[\nu_i^{-(M-\gamma)} - \nu_i^{-M} r_{\gamma,k}(\nu_i)\right]^2 (\Psi_i, \mathbf{f})^2$$

$$\leq \left(\mu_1^{M-\gamma}\right)^2 \max_{\nu_i} \left[\nu_i^{-M}\left(\nu_i^{\gamma} - r_{\gamma,k}(\nu_i)\right)\right]^2 \sum_{i=1}^{n} (\Psi_i, \mathbf{f})^2$$

$$\leq \left(\mu_1^{M-\gamma}\right)^2 (\kappa(\mathbb{A}))^{2M}\, E^2_{\beta,k} ||\mathbf{f}||^2_{\ell_2},$$

where $\nu_i^{-1} \leq \kappa(\mathbb{A})$ is used. Finally

$$||\mathbf{u}-\underline{\mathbf{w}}||_{\ell_2} \leq C_\gamma \mu_1^{M-\gamma} \kappa^M(\mathbb{A})\; e^{-2\pi\sqrt{k\gamma}} ||\mathbf{f}||_{\ell_2}, \tag{4.3}$$

which completes the proof. □

As with the previous theorems, the following corollary is true.

Corollary 3 *For every arbitrary small $\epsilon > 0$, there exits integer k such that*

$$||\mathbf{v}-\underline{\mathbf{v}}||_{\ell_2} \leq (1+\epsilon)\mu_1^{\alpha} \kappa^{\lceil\alpha\rceil}(\mathbb{A})\; e^{-2\pi\sqrt{k(\lceil\alpha\rceil-\alpha)}} 4^{1+(\lceil\alpha\rceil-\alpha)} |\sin\pi(\lceil\alpha\rceil-\alpha)|\; ||\mathbf{f}||_{\ell_2}. \tag{4.4}$$

Unlike the case of solving systems with $\mathbb{A}^\alpha$, the estimate here depends on the condition number of $\mathbb{A}$. At the same time, it is worth noting that for a given matrix the error exponentially decreases as k increases.

4.2 Comparative analysis.

Here, we consider the discussed BURA-based method for $\alpha \in (0,1)$. This case is currently of primary interest due to the fact that such matrix-vector multiplications naturally arise in the solution of time-dependent problems, including a sub-diffusive elliptic term. As in the similar study in Section 3.3, we assume that $\mu_1 = 1$. Thus, for $\alpha \in \{0.25, 0.5, 0.75\}$, the estimate (4.4) leads to the following asymptotic bounds of the relative errors:

- $\alpha = 0.25$:

$$\frac{||\mathbf{v}-\underline{\mathbf{v}}||_{\ell_2}}{||\mathbf{f}||_{\ell_2}} \approx 4\kappa(\mathbb{A}) e^{-\pi\sqrt{3k}} \tag{4.5}$$

- $\alpha = 0.5$:

$$\frac{||\mathbf{v}-\underline{\mathbf{v}}||_{\ell_2}}{||\mathbf{f}||_{\ell_2}} \approx 8\kappa(\mathbb{A}) e^{-\pi\sqrt{2k}} \tag{4.6}$$

- $\alpha = 0.75$:

$$\frac{||\mathbf{v}-\underline{\mathbf{v}}||_{\ell_2}}{||\mathbf{f}||_{\ell_2}} \approx 4\kappa(\mathbb{A}) e^{-\pi\sqrt{k}} \tag{4.7}$$

4.3 Best uniform rational approximation of z^α, $z \in [1, \bar{\kappa}]$ and BRASIL based experimental study.

We follow the notation from previous section, that is $\bar{\kappa} \geq \kappa(\mathbb{A})$. Here we consider the best uniform rational approximation $\check{r}_{\alpha,k,\bar{\kappa}}$ of z^α, $z \in [1, \bar{\kappa}]$ defined as

$$\check{r}_{\alpha,k,\bar{\kappa}}(z) := \underset{r_k(z)\in\mathcal{R}_k}{\operatorname{argmin}} \max_{z\in[1,\bar{\kappa}]} |r_k(z) - z^\alpha|. \tag{4.8}$$

In this case the error reads as

$$\check{E}_{\alpha,k,\bar{\kappa}} := \max_{z\in[1,\bar{\kappa}]} |\check{r}_{\alpha,k,\bar{\kappa}}(z) - z^\alpha|. \tag{4.9}$$

Now we introduce the approximation $\check{\mathbf{v}}$ of $\mathbf{v}$,

$$\check{\mathbf{v}} := \mu_1^{-\alpha} \check{r}_{\alpha,k,\delta}(\frac{1}{\mu_1}\mathbb{A})\mathbf{f}. \tag{4.10}$$

Lemma 2 *For each $\alpha \in \mathbb{R}^+ \setminus \mathbb{Z}$, the approximation $\check{\mathbf{v}}$ of $\mathbf{v} = \mathbb{A}^\alpha(f)$ satisfies the error estimate*

$$||\mathbf{v} - \check{\mathbf{v}}||_{\ell_2} \leq \mu_1^\alpha \check{E}_{\alpha,k,\bar{\kappa}} ||\mathbf{f}||_{\ell_2}. \tag{4.11}$$

Proof The approach is rather similar to the proof of Lemma 1:

$$\mathbf{f} = \sum_{i=1}^{n} (\Psi_i, \mathbf{f})\Psi_i,$$

$$\mathbf{v} = \mu_1^\alpha \sum_{i=1}^{n} \left(\frac{\mu_i}{\mu_1}\right)^\alpha (\Psi_i, \mathbf{f})\Psi_i = \mu_1^\alpha \sum_{i=1}^{n} \hat{\nu}_i^\alpha (\Psi_i, \mathbf{f})\Psi_i,$$

$$\check{\mathbf{v}} = \mu_1^\alpha \sum_{i=1}^{n} \check{r}_{\alpha,k,\bar{\kappa}} \left(\frac{\mu_i}{\mu_1}\right) (\Psi_i, \mathbf{f})\Psi_i = \mu_1^\alpha \sum_{i=1}^{n} \check{r}_{\alpha,k,\bar{\kappa}}(\hat{\nu}_i)(\Psi_i, \mathbf{f})\Psi_i,$$

$\hat{\nu}_i := \mu_i/\mu_1 \in [1, \kappa(\mathbb{A})] \subset [1, \bar{\kappa}]$. Therefore

$$\begin{aligned} ||\mathbf{v} - \check{\mathbf{v}}||_{\ell_2}^2 &= \mu_1^{2\alpha} \sum_{i=1}^{n} \left(\hat{\nu}_i^\alpha - \check{r}_{\alpha,k,\bar{\kappa}}(\hat{\nu}_i)\right)^2 (\Psi_i, \mathbf{f})^2 \\ &\leq \mu_1^{2\alpha} \max_{\hat{\nu}_i} |\hat{\nu}_i^\alpha - \check{r}_{\alpha,k,\bar{\kappa}}(\hat{\nu}_i)|^2 \sum_{i=1}^{n} (\Psi_i, \mathbf{f})^2 \\ &= \mu_1^{2\alpha} \check{E}_{\alpha,k,\bar{\kappa}}^2 ||\mathbf{f}||_{\ell_2}^2, \end{aligned}$$

which completes the proof. □

Again, BRASIL [33] is used to perform a set of numerical tests where $\check{r}_{\alpha,k,\bar{\kappa}}$ and $\check{E}_{\alpha,k,\bar{\kappa}}$ are computed. For direct comparison with (4.5), (4.6) and (4.7), we assume that $\mu_1 = 1$, $\bar{\kappa} = \kappa(\mathbb{A})$, and run test problems for $\alpha \in \{0.25, 0.5, 0.75\}$ and $\bar{\kappa} \in \{10^4, 10^6, 10^8, 10^{12}, 10^{14}\}$, varying the degree $k \in \{4, 8, 12, 16, 20, 24\}$.

As well as in the previous section, we are also interested in the behaviour of the poles of $\check{r}_{\alpha,k,\bar{\kappa}}$.

Detailed information about the errors $\check{E}_{\alpha,k,\bar{\kappa}}$ of the best uniform rational approximation $\check{r}_{\alpha,k,\bar{\kappa}}$ computed by BRASIL is presented in Table 1. The behaviour is complex, and as expected, the accuracy depends nonlinearly on k, α, and $\bar{\kappa}$. A general observation is that larger α and larger $\bar{\kappa}$ have a cumulative effect leading to an increase in error. The data presented can be used as a practical guide for choosing the minimum degree k required to achieve a given accuracy for a given problem. So, for example, bold numbers indicate the row to the right of which the error is greater than 10^{-2}. Therefore, if this is the desired accuracy, k should be chosen large enough so that we are to the left of this line.

α	$k \setminus \bar{\kappa}$	10^6	10^8	10^{10}	10^{12}	10^{14}
0.25	4	0.0717879	0.4081965	1.5929635	5.3930242	17.426749
0.25	8	**0.0006294**	0.0100670	0.0733356	0.3482379	1.3030811
0.25	12	5.433E-06	0.0002446	**0.0034735**	0.0262502	0.1353156
0.25	16	4.672E-08	5.920E-06	0.0001635	**0.0019666**	0.0142936
0.25	20	4.011E-10	1.430E-07	7.682E-06	0.0001469	0.0015038
0.25	24	3.444E-12	3.451E-09	3.606E-07	1.097E-05	0.0001580
0.50	4	0.6066483	7.2019398	73.487885	736.39463	7365.4671
0.50	8	**0.0051205**	0.1460175	1.9760122	20.730924	2085.0364
0.50	12	0.0000439	**0.0035143**	0.0888404	1.2199808	12,12.945
0.50	16	3.758E-07	8.469E-05	**0.0041613**	0.0891009	1.1721118
0.50	20	3.219E-09	2.041E-06	0.0001950	**0.0066353**	0.1209103
0.50	24	2.768E-11	4.919E-08	9.139E-06	**0.0004943**	0.0136298
0.75	4	3.0330156	99.393589	3147.5719	99539.733	3147727.6
0.75	8	0.0213472	1.1587447	38.756285	1228.6761	38857.543
0.75	12	**0.0001793**	0.0257681	1.2302894	40.654230	1288.1467
0.75	16	1.524E-06	**0.0006128**	0.0540855	2.2213180	71.933281
0.75	20	1.301E-08	1.468E-05	**0.0025040**	0.1537364	5.5821657
0.75	24	1.130E-10	3.527E-07	**0.0001167**	0.0112863	0.5282139

Table 1 Errors $\check{E}_{\alpha,k,\bar{\kappa}}$ computed by BRASIL.

The graphs in Fig. 2 and 3 show the behaviour of $\check{E}_{\alpha,k,\bar{\kappa}}$ for $\alpha = 0.5$ and $k \in \{4, 6, 8, 10, 12\}$. Errors obtained by estimate (4.6) (Fig. 2) and those computed by BRASIL (Fig. 3) are compared. In both cases, we clearly see the exponential convergence rate with respect to k. We also observe a strong advantage of the best rational approximation $\check{r}_{0.5,k,\bar{\kappa}}$ computed by BRASIL.

In estimate (4.11), $\check{E}_{\alpha,k,\bar{\kappa}}$ grows linearly as $\kappa(\mathbb{A})$ increases. However, the data in Table 1 may provoke the question of whether the growth is always linear. For example, for $\alpha = 0.5$ and $k = 4$ we see a factor similar to $\kappa^{\alpha}(\mathbb{A})$ in $\check{E}_{\alpha,k,\bar{\kappa}}$ when $\bar{\kappa} \in \{10^8, 10^{10}, 10^{12}, 10^{14}\}$. This issue is addressed in Fig. 4 where the plots for $\alpha \in \{0.25, 05, 0.75\}$ are shown. In all cases, we see how the error growth becomes increasingly closer to linear for sufficiently large $\bar{\kappa}$.

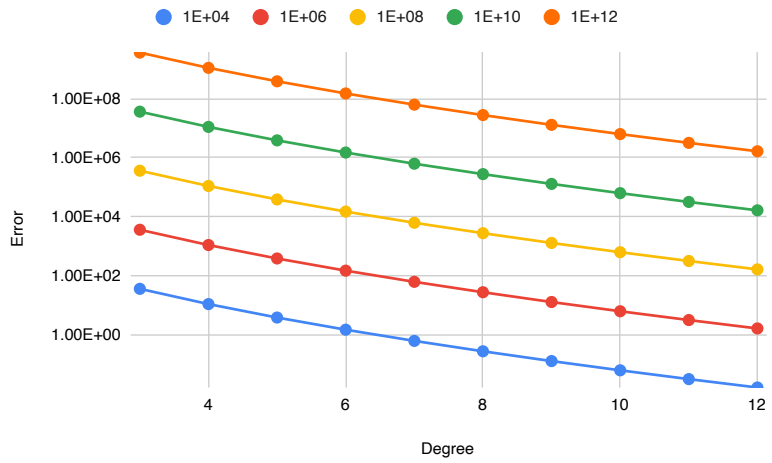

Fig. 2 Errors $\check{E}_{0.5,12,\bar{\kappa}}$ versus degree $k \in \{4,6,8,10,12\}$ for $\bar{\kappa} \in \{10^4, 10^6, 10^8, 10^{10}, 10^{12}\}$ estimated by (4.6).

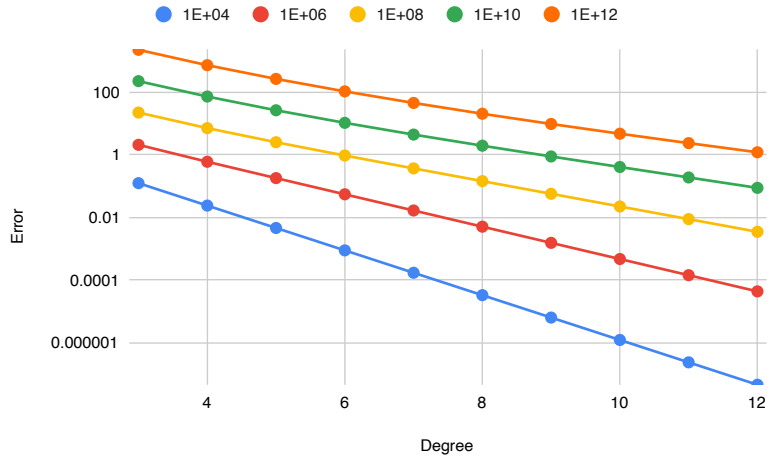

Fig. 3 Errors $\check{E}_{0.5,12,\bar{\kappa}}$ versus degree $k \in \{4,6,8,10,12\}$ for $\bar{\kappa} \in \{10^4, 10^6, 10^8, 10^{10}, 10^{12}\}$ computed by BRASIL.

5 Concluding remarks

This paper presents a general approach to solving problems involving fractional powers of sparse SPD matrices, accompanied by systematic theoretical and experimental error analysis.

The proposed methods and algorithms for approximation of $\mathbb{A}^{-\alpha}$ and $\mathbb{A}^{\alpha}$ for arbitrary $\alpha > 0$ significantly extends the results of [20,22]. The resulting

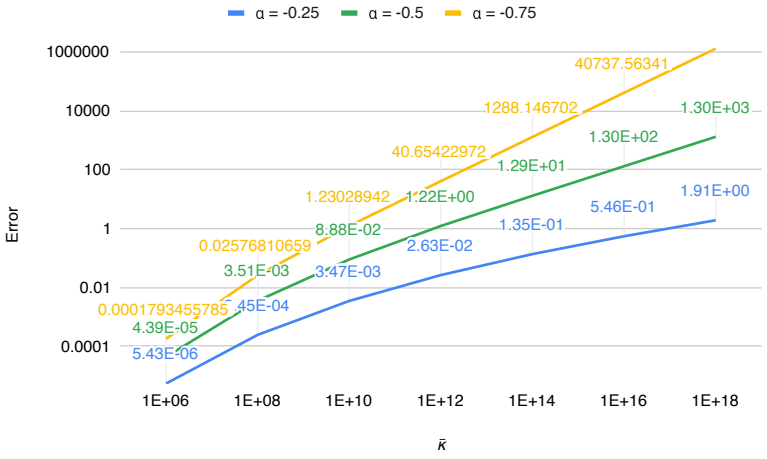

Fig. 4 Errors $\check{E}_{\alpha,12,\bar{\kappa}}$ computed by BRASIL versus $\bar{\kappa} \in \{10^6, 10^8, 10^{10}, 10^{12}, 10^{14}, 10^{16}, 10^{18}\}$.

BURA and BURA-based methods have an exponential rate of convergence with respect to power k, regardless of the condition number $\kappa(\mathbb{A})$. The methods and algorithms for matrix-vector multiplication with $\mathbb{A}^\alpha$ also have an exponential rate of convergence with respect to k for a given upper bound $\bar{\kappa} \geq \kappa(\mathbb{A})$. However, theoretical estimates and numerical experiments show that the error grows linearly with $\bar{\kappa}$. Thus, it turns out that matrix-vector multiplication is a more complex problem than solving systems with $\mathbb{A}^\alpha$. This conclusion is consistent with related results on multigrid methods for discrete fractional Sobolev spaces [5] and the discussions in [19].

The algorithmic implementation of the BURA method introduced in [20] fundamentally exploits the interlacing property of real roots and poles of the best uniform rational approximation of z^α on $[0, 1]$ for $\alpha \in (0, 1)$. In the general case of positive or negative α, we need a detailed consideration of this issue, which is beyond the scope of the present paper. Such a question does not apply to BURA-based variants, which are superposition of a certain integer degree of $\mathbb{A}$ and BURA for $\alpha \in (0, 1)$. In this sense, we note some advantages of BURA-based methods, although their accuracy is relatively lower.

All the methods discussed in this study reduce the non-local problem to a set of auxiliary linear systems with sparse SPD matrices. The additive BURA-AR and multiplicative BURA-MR methods introduced in [18] follow the observation that the sparse SPD matrices involved possess extremely different properties. As a result, solution methods with improved computational complexity are developed. Although significantly different in origin, the results recently published in [28] relate to the same phenomenon. In [18,28], $\alpha \in (0, 1)$. The importance of this topic is enhanced in the context of the new results presented here. This is especially true in the case of negative α (or matrix-vector

multiplication), where larger k are needed to compensate for the influence of $\kappa(\mathbb{A})$.

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Conflict of interest

The authors declare that they have no conflict of interest.

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