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A GAUSS-LAGUERRE APPROACH FOR THE RESOLVENT OF FRACTIONAL POWERS*

ELEONORA DENICH†, LAURA GRAZIA DOLCE†, AND PAOLO NOVATI†

Abstract. This paper introduces a very fast method for the computation of the resolvent of fractional powers of operators. The analysis is kept in the continuous setting of (potentially unbounded) self-adjoint positive operators in Hilbert spaces. The method is based on the Gauss-Laguerre rule, exploiting a particular integral representation of the resolvent. We provide sharp error estimates that can be used to a priori select the number of nodes to achieve a prescribed tolerance.

Key words. resolvent of fractional powers, Gauss-Laguerre rule, functions of operators

AMS subject classifications. 47A58, 65F60, 65D32

1. Introduction.

Let $\mathcal{H}$ be a Hilbert space with inner product $\langle \cdot, \cdot \rangle$ and induced norm $\| \cdot \|$. In this work we are interested in the computation of the resolvent of the fractional power

$$\mathcal{R}_{h,\alpha}(\mathcal{L}) = (I + h\mathcal{L}^{\alpha})^{-1},$$

where $h > 0$, $0 < \alpha < 1$, I is the identity operator, and $\mathcal{L} : \mathcal{H} \to \mathcal{H}$ is a self-adjoint, positive operator. The problem finds application in the solution of fractional-in-space parabolic equations like

$$\frac{\partial U}{\partial t} = \Delta_{\alpha} U + F,$$

where Δ_{α} denotes the fractional Laplacian that can be defined following the rule of the operational calculus as $\Delta_{\alpha} = -(-\Delta)^{\alpha}$, in which Δ is the Laplace operator with suitable boundary conditions. In the above equation, F represents a generic forcing term. Starting from the spectral decomposition of Δ, the operation $(-\Delta)^{\alpha}$ is obtained by simply raising to the power α the eigenvalues of $-\Delta$. Denoting by $A \in \mathbb{R}^{N \times N}$ a general symmetric positive definite discretization of $-\Delta$, the use of an implicit time stepping procedure leads to the computation of one or more matrix functions of the type $\mathcal{R}_{h,\alpha}(A)$, where $h > 0$ is a parameter that typically depends on the time step and on the coefficients of the integrator.

Going back to a generic $\mathcal{L} \colon \mathcal{H} \to \mathcal{H}$, clearly the numerical approximation of $\mathcal{R}_{h,\alpha}(\mathcal{L})$ requires the discretization of $\mathcal{L}$. Anyway, since we want to keep the analysis independent of the type and the sharpness of the discretization, we prefer to work in the infinite-dimensional setting of an operator $\mathcal{L}$, with spectrum $\sigma(\mathcal{L})$ contained in $[a, +\infty)$, $a > 0$, thus potentially unbounded. Since we do not introduce any restriction on the magnitude of h, without loss of generality throughout the paper we assume for simplicity $a = 1$.

The numerical approach considered in this work employs a particular integral representation of the function $\mathcal{R}_{h,\alpha}(\lambda) = (1 + h\lambda^{\alpha})^{-1}$. With some manipulations explained in Section 2, the representation allows us to write $\mathcal{R}_{h,\alpha}(\lambda)$ as the sum of two integrals, that is,

$$\mathcal{R}_{h,\alpha}(\lambda) = \frac{\sin(\alpha\pi)}{\alpha\pi} \left(I^{(1)}(\lambda) + I^{(2)}(\lambda) \right), \tag{1.1}$$

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†Dipartimento di Matematica e Geoscienze, Università di Trieste, Trieste, Italy
(`eleonora.denich@phd.units.it`, `lauragrazia.dolce@studenti.units.it`, `novati@units.it`).

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with

$$I^{(1)}(\lambda) := \int_0^{+\infty} \frac{e^{-x}}{\left(1 + e^{-\frac{x}{\alpha}} h^{\frac{1}{\alpha}} \lambda\right)(e^{-2x} + 2e^{-x}\cos(\alpha\pi) + 1)} dx, \tag{1.2}$$

$$I^{(2)}(\lambda) := \int_0^{+\infty} \frac{\alpha(\alpha+1)^{-1} e^{-x}}{\left(e^{-\frac{x}{\alpha+1}} + h^{\frac{1}{\alpha}} \lambda\right)\left(e^{-\frac{2\alpha x}{\alpha+1}} + 2e^{-\frac{\alpha x}{\alpha+1}}\cos(\alpha\pi) + 1\right)} dx, \tag{1.3}$$

which we evaluate by using the n-point Gauss-Laguerre rule. This formula leads to a rational approximation $R_{2n-1,2n}(\lambda) \cong \mathcal{R}_{h,\alpha}(\lambda)$, where $R_{2n-1,2n} = p_{2n-1}/q_{2n}$, $p_{2n-1} \in \Pi_{2n-1}$, $q_{2n} \in \Pi_{2n}$. Here and below we use the symbol $\cong$ to indicate a generic approximation. Finally, we thus obtain

$$\mathcal{R}_{h,\alpha}(\mathcal{L}) \cong R_{2n-1,2n}(\mathcal{L}),$$

in which the degree $2n$ of the denominator also represents the number of inversions of suitable shifts of the operator $\mathcal{L}$.

Thanks to the existing error estimates based on the theory of analytic functions, we are able to derive sharp error estimates for the operator case. This is possible because $(\sigma(\mathcal{L}) \subseteq [1, +\infty))$

$$\|\mathcal{R}_{h,\alpha}(\mathcal{L}) - R_{k-1,k}(\mathcal{L})\|_{\mathcal{H}\to\mathcal{H}} \leq \max_{\lambda\in[1,+\infty)} |\mathcal{R}_{h,\alpha}(\lambda) - R_{2n-1,2n}(\lambda)|, \tag{1.4}$$

where $\|\cdot\|_{\mathcal{H}\to\mathcal{H}}$ is the induced operator norm. The bound (1.4) allows us to study the error by working in a scalar setting. This analysis shows that, by using the same number n of Gauss-Laguerre points for both integrals, the error decays like

$$\exp\left(-\text{const} \cdot n^{1/3}\right).$$

Nevertheless, exploiting the sharpness of the estimates, we are able to remarkably improve the efficiency of the method by balancing the error contributions of the two integrals, together with a suitable truncation of the Gauss-Laguerre rule. In this way we show that the error decays like

$$\exp\left(-\text{const} \cdot q^{1/2}\right),$$

where $q \ll 2n$ represents the number of inversions.

We remark that the analysis given in the paper is rather complicated, and we have been forced to use a number of approximations which are sometimes the consequence of experimental evidences. Nevertheless, the final estimates appear to be very accurate, and this, somehow, justifies our choices.

The computation of the resolvent $\mathcal{R}_{h,\alpha}(\mathcal{L})$, where $\mathcal{L}$ is an unbounded operator, has already been studied in [3]. The particular case of $\mathcal{L}$ representing a matrix has been considered in [14], where the shift-and-invert Krylov method is employed, and in [1], where the rational Krylov method based on the use of zeros of the Jacobi polynomials is considered. We remark that the approach proposed here can also be employed to define the poles of a rational Krylov method. Since $\mathcal{R}_{h,\alpha}(\lambda) \sim \frac{1}{h}\lambda^{-\alpha}$, for $\lambda \to +\infty$ (the symbol $\sim$ denotes asymptotic equivalence), in principle one may use the poles of a rational approximation of $\lambda^{-\alpha}$ (see, e.g., [2, 6, 7, 8, 9, 10, 11, 12, 17, 18, 19]) also for $\mathcal{R}_{h,\alpha}(\lambda)$. Clearly, working directly with $\mathcal{R}_{h,\alpha}(\lambda)$ allows one to obtain better results.

This work is organized as follows. In Section 2 we derive the used integral representation, and we describe the Gauss-Laguerre method. In Section 3 we study the error in the scalar case. In Section 4 we extend the analysis to the operator case. Finally, in Sections 5 and 6 we present some improvements based on the properties of the integrand functions and on the asymptotic behavior of the Gauss-Laguerre weights.

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2. The Gauss-Laguerre method. Let $\lambda \in \mathbb{C}\backslash(-\infty,0]$, and consider the Cauchy integral representation

$$\mathcal{R}_{h,\alpha}(\lambda) = \frac{1}{2\pi i}\int_{\Gamma}(z-\lambda)^{-1}(1+hz^{\alpha})^{-1}dz,$$

where Γ is a contour in $\mathbb{C}\setminus(-\infty,0)$ containing λ in its interior. The first step for the construction of our method is to select Γ as the boundary of the sector of the complex plane with semiangle $\alpha\pi$ and vertex at the origin, that is,

$$\Gamma = \Gamma_{\alpha} := \Gamma_{\alpha}^{+} \cup \Gamma_{\alpha}^{-},$$

where $\Gamma_{\alpha}^{\pm} = \{w | w = \rho e^{\pm i\alpha\pi}, \rho \geq 0\}$. Then, the change of variable $z = \left(\frac{w}{h}\right)^{1/\alpha}$ leads to

$$\mathcal{R}_{h,\alpha}(\lambda) = \frac{1}{2\pi i\alpha h^{\frac{1}{\alpha}}}\int_{\Gamma_{\alpha}} \frac{1}{\left(w^{\frac{1}{\alpha}}h^{-\frac{1}{\alpha}}-\lambda\right)(1+w)} w^{\frac{1}{\alpha}-1}dw.$$

Now, defining $w = \rho e^{i\pi\alpha}$ for $w \in \Gamma_{\alpha}^{+}$, $w = \rho e^{-i\pi\alpha}$ for $w \in \Gamma_{\alpha}^{-}$, and running Γ_{α} in the counterclockwise direction, we obtain

$$\begin{aligned}\mathcal{R}_{h,\alpha}(\lambda) &= \frac{1}{2\pi i\alpha h^{\frac{1}{\alpha}}}\left[-\int_0^{+\infty}\frac{\rho^{\frac{1}{\alpha}}e^{i\pi}e^{i\alpha\pi}}{\rho e^{i\pi\alpha}\left(\rho^{\frac{1}{\alpha}}e^{i\pi}h^{-\frac{1}{\alpha}}-\lambda\right)(1+\rho e^{+i\alpha\pi})}d\rho\right.\\ &\qquad\left.+\int_0^{+\infty}\frac{\rho^{\frac{1}{\alpha}}e^{-i\pi}e^{-i\alpha\pi}}{\rho e^{-i\pi\alpha}\left(\rho^{\frac{1}{\alpha}}e^{-i\pi}h^{-\frac{1}{\alpha}}-\lambda\right)(1+\rho e^{-i\alpha\pi})}d\rho\right]\\ &= \frac{\sin(\alpha\pi)}{\alpha\pi}\int_0^{+\infty}\frac{\rho^{\frac{1}{\alpha}}}{\left(\rho^{\frac{1}{\alpha}}+h^{\frac{1}{\alpha}}\lambda\right)(1+2\rho\cos(\alpha\pi)+\rho^2)}d\rho. \qquad (2.1)\end{aligned}$$

We remark that the integral representation (2.1), with λ replaced by a regularly accretive operator $\mathcal{L}$, was derived by Kato in [15]. Now, by the change of variable $\rho = e^{y}$, we obtain

$$\begin{aligned}\mathcal{R}_{h,\alpha}(\lambda) &= \frac{\sin(\alpha\pi)}{\alpha\pi}\int_{-\infty}^{+\infty}\frac{e^{\frac{\alpha+1}{\alpha}y}}{\left(e^{\frac{y}{\alpha}}+h^{\frac{1}{\alpha}}\lambda\right)(1+2\cos(\alpha\pi)e^{y}+e^{2y})}dy\\ &= \frac{\sin(\alpha\pi)}{\alpha\pi}\left[\int_0^{+\infty}\frac{e^{-y}}{\left(1+e^{\frac{-y}{\alpha}}h^{\frac{1}{\alpha}}\lambda\right)(e^{-2y}+2\cos(\alpha\pi)e^{-y}+1)}dy\right.\\ &\qquad\left.+\int_{-\infty}^{0}\frac{e^{\frac{\alpha+1}{\alpha}y}}{\left(e^{\frac{y}{\alpha}}+h^{\frac{1}{\alpha}}\lambda\right)(1+2\cos(\alpha\pi)e^{y}+e^{2y})}dy\right].\end{aligned}$$

Using for the second integral the further change of variable $-x = \frac{\alpha+1}{\alpha}y$, we finally obtain equation (1.1), in which the integrals (see (1.2) and (1.3)) can be written as

$$I^{(i)}(\lambda) = \int_0^{+\infty} e^{-x}f_i(x)dx, \quad i = 1,2,$$

with

$$f_1(x) := \left(1+e^{\frac{-x}{\alpha}}h^{\frac{1}{\alpha}}\lambda\right)^{-1}\left(e^{-2x}+2e^{-x}\cos(\alpha\pi)+1\right)^{-1}, \qquad (2.2)$$

$$f_2(x) := \frac{\alpha}{\alpha+1}\left(e^{\frac{-x}{\alpha+1}}+h^{\frac{1}{\alpha}}\lambda\right)^{-1}\left(1+2\cos(\alpha\pi)e^{\frac{-\alpha x}{\alpha+1}}+e^{\frac{-2\alpha x}{\alpha+1}}\right)^{-1}. \qquad (2.3)$$

REMARK 2.1. The functions f_1 and f_2 depend on λ in the scalar case or on $\mathcal{L}$ in the operator case. To keep the notation as simple as possible, we omit this dependence since it is always clear from the context.

Remembering that we assume $\sigma(\mathcal{L}) \subseteq [1, +\infty)$, we restrict our considerations to the case $\lambda \geq 1$. In this situation, we observe that for $x \in [0, +\infty)$ we have $0 \leq f_i(x) \leq K_i$, $i = 1, 2$, where

$$K_1 = 1 \quad \text{and} \quad K_2 = \frac{\alpha}{\alpha + 1} h^{-\frac{1}{\alpha}}. \tag{2.4}$$

By using the Gauss-Laguerre rule, we then approximate the resolvent (cf. (1.1)) by

$$\mathcal{R}_{h,\alpha}(\lambda) \cong \frac{\sin(\alpha\pi)}{\alpha\pi} \left[I_n^{(1)}(\lambda) + I_n^{(2)}(\lambda) \right], \quad \text{where} \quad I_n^{(i)}(\lambda) := \sum_{j=1}^{n} w_j^{(n)} f_i(x_j^{(n)}), \tag{2.5}$$

in which $x_j^{(n)}$ and $w_j^{(n)}$, for $j = 1, \ldots, n$, are, respectively, the nodes and the weights of the n-point Gauss-Laguerre rule. In the sequel we denote by

$$e_n^{(i)} := I^{(i)}(\lambda) - I_n^{(i)}(\lambda), \quad i = 1, 2, \tag{2.6}$$

the corresponding errors. Clearly, (2.5) is actually a rational approximation of type

$$\mathcal{R}_{h,\alpha}(\lambda) \cong R_{2n-1,2n}(\lambda) = \frac{p_{2n-1}(\lambda)}{q_{2n}(\lambda)}, \qquad p_{2n-1} \in \Pi_{2n-1},\ q_{2n} \in \Pi_{2n}.$$

3. Error estimates in the scalar case. Let f be a generic function, analytic in a region of the complex plane containing the positive real axis. Let

$$I(f) = \int_0^{+\infty} e^{-x} f(x) dx$$

and $I_n(f)$ be the n-point Gauss-Laguerre rule. In order to estimate $e_n(f) = I(f) - I_n(f)$, we employ the theory introduced in [5]. Let us define for any $\mathcal{S} > 1$ the parabola $\Gamma_{\mathcal{S}}$ in the complex plane given by

$$\mathfrak{Re}(\sqrt{-z}) = \ln(\mathcal{S}). \tag{3.1}$$

$\Gamma_{\mathcal{S}}$ is symmetric with respect to the real axis, it has convexity oriented towards the positive real axis, and a vertex at $-(\ln(\mathcal{S}))^2$. By writing $z = a + ib$, equation (3.1) becomes

$$\sqrt{\frac{\sqrt{a^2 + b^2} - a}{2}} = \ln(\mathcal{S}),$$

and thus we can rewrite the parabola in Cartesian coordinates as

$$a = \left(b^2 - 4(\ln(\mathcal{S}))^4\right) \frac{1}{4(\ln(\mathcal{S}))^2}. \tag{3.2}$$

Observe that for $\mathcal{S} \to 1$ the parabola degenerates to the positive real axis.

Suppose that for a certain $\mathcal{S}$ the function f is analytic on and within $\Gamma_{\mathcal{S}}$ except for a pair of simple poles z_0 and its conjugate $\overline{z}_0$. Then, the error can be estimated as follows (see [5]):

$$e_n(f) \cong -4\pi \mathfrak{Re} \left\{ r(f; z_0) e^{-z_0} \left(e^{\sqrt{-z_0}} \right)^{-2\sqrt{\overline{n}}} \right\}, \tag{3.3}$$

where $\overline{n} = 4n + 2$ and $r(f; z_0)$ is the residue of f at z_0. Let $\mathcal{S}_0 > 1$ be such that z_0 and $\overline{z}_0$ belong to $\Gamma_{\mathcal{S}_0}$. Then, by (3.1) and (3.3) we have that

$$|e_n(f)| \cong \text{const} \cdot \mathcal{S}_0^{-2\sqrt{\overline{n}}}. \tag{3.4}$$

3.1. Poles and residues. In order to employ the above theory to estimate the error of the approximation (2.5), we have to study the poles and residues of the functions $f_1(z)$ and $f_2(z)$; see (2.2) and (2.3). For both functions, the key point is to understand the poles closest to $[0, +\infty)$, where the distance is expressed by $\mathcal{S}_0$; see (3.4). For simplicity, we define the auxiliary functions

$$a^{(I)}(z) := 1 + e^{\frac{-z}{\alpha}} h^{\frac{1}{\alpha}} \lambda, \qquad a^{(II)}(z) := e^{-2z} + 2e^{-z}\cos(\alpha\pi) + 1,$$
$$a^{(III)}(z) := e^{\frac{-z}{\alpha+1}} + h^{\frac{1}{\alpha}} \lambda, \qquad a^{(IV)}(z) := 1 + 2\cos(\alpha\pi) e^{\frac{-\alpha z}{\alpha+1}} + e^{\frac{-2\alpha z}{\alpha+1}},$$

so that

$$f_1(z) = \left[a^{(I)}(z) a^{(II)}(z)\right]^{-1}, \qquad f_2(z) = \frac{\alpha}{\alpha+1}\left[a^{(III)}(z) a^{(IV)}(z)\right]^{-1}.$$

3.1.1. The first integral. The poles of f_1 are obtained by solving $a^{(I)}(z)a^{(II)}(z) = 0$. Starting from $a^{(I)}(z) = 0$ we obtain the set

$$z_k^{(I)} := \alpha \ln(h^{\frac{1}{\alpha}} \lambda) + i(2k+1)\alpha\pi, \quad k \in \mathbb{Z}.$$

The points closest to $[0, +\infty)$ are therefore

$$z_0^{(I)} = \alpha \ln(h^{\frac{1}{\alpha}} \lambda) + i\alpha\pi \tag{3.5}$$

and its conjugate, obtained for $k = 0$ and $k = -1$. As for the poles arising from $a^{(II)}(z)$, we obtain

$$z_k^{(II)} := i(2k + 1 \pm \alpha)\pi, \quad k \in \mathbb{Z},$$

and now the closest ones to the real axis are

$$z_0^{(II)} = i(1-\alpha)\pi \tag{3.6}$$

and its conjugate. In order to estimate the error $e_n^{(1)}(\lambda)$ (see (2.6)), let $\Gamma_{\mathcal{S}_0^{(II)}}$ be the parabola passing through the pole $z_0^{(II)}$. If it contains $z_0^{(I)}$ in its interior, then we use the error formula (3.3) with $z_0 = z_0^{(I)}$, otherwise with $z_0 = z_0^{(II)}$. By using the Cartesian expression (3.2), it is rather easy to demonstrate that $z_0^{(I)}$ is inside $\Gamma_{\mathcal{S}_0^{(II)}}$ for

$$\ln\left(h^{\frac{1}{\alpha}} \lambda\right) > \frac{(2\alpha - 1)\pi}{2\alpha(1-\alpha)}. \tag{3.7}$$

Defining

$$\overline{\lambda} := \exp\left(\frac{(2\alpha-1)\pi}{2\alpha(1-\alpha)}\right) h^{-\frac{1}{\alpha}}, \tag{3.8}$$

we simply write $\lambda > \overline{\lambda}$ to express condition (3.7). We remark that, depending on h and α, this condition may be verified for each $\lambda \geq 1$, or eventually, only for λ sufficiently large.

As for the residues of f_1 at $z_0^{(I)}$ and $z_0^{(II)}$, after some computations one finds

$$r(f_1; z_0^{(I)}) = \frac{1}{a^{(II)}(z_0^{(I)})} \lim_{z \to z_0^{(I)}} \frac{z - z_0^{(I)}}{a^{(I)}(z)} = \frac{\alpha h^2 \lambda^{2\alpha}}{e^{-2i\alpha\pi} + 2h\lambda^{\alpha}\cos(\alpha\pi)e^{-i\alpha\pi} + h^2\lambda^{2\alpha}}$$

and

$$r(f_1; z_0^{(II)}) = \frac{1}{a^{(I)}(z_0^{(II)})} \lim_{z \to z_0^{(II)}} \frac{z - z_0^{(II)}}{a^{(II)}(z)} = \frac{ie^{-i\alpha\pi}}{2\sin(\alpha\pi)\left(1 - e^{-i\frac{\pi}{\alpha}} h^{\frac{1}{\alpha}} \lambda\right)}.$$

3.1.2. The second integral. Following the same steps of Section 3.1.1, we obtain the poles of f_2 by solving $a^{(III)}(z)a^{(IV)}(z) = 0$. Starting from $a^{(III)}(z) = 0$ we find the set

$$z_k^{(III)} := -(\alpha+1)\ln(h^{\frac{1}{\alpha}}\lambda) + i(2k+1)(\alpha+1)\pi, \quad k \in \mathbb{Z},$$

and the closest points to the real axis are

$$z_0^{(III)} = -(\alpha+1)\ln(h^{\frac{1}{\alpha}}\lambda) + i(\alpha+1)\pi \tag{3.9}$$

and its conjugate. By solving $a^{(IV)}(z) = 0$ we obtain

$$z_k^{(IV)} := i(2k+1\pm\alpha)\frac{\alpha+1}{\alpha}\pi, \quad k \in \mathbb{Z},$$

and now the closest ones are

$$z_0^{(IV)} = i\frac{(1-\alpha)(\alpha+1)}{\alpha}\pi \tag{3.10}$$

and its conjugate. Analogously to the first integral, we have to compare the parabolas passing through $z_0^{(III)}$ and $z_0^{(IV)}$. With some computations it is not difficult to see that $z_0^{(III)}$ is inside the parabola $\Gamma_{\mathcal{S}_0^{(IV)}}$ passing though $z_0^{(IV)}$ if

$$\ln\left(h^{\frac{1}{\alpha}}\lambda\right) < -\frac{(2\alpha-1)\pi}{2\alpha(1-\alpha)}.$$

It may happen that the above condition is not satisfied for any $\lambda \geq 1$. Hence, it must be replaced by

$$1 \leq \lambda < \bar{\bar{\lambda}}, \quad \text{where} \quad \bar{\bar{\lambda}} = \max\left\{1, e^{-\frac{(2\alpha-1)\pi}{2\alpha(1-\alpha)}}h^{-\frac{1}{\alpha}}\right\}. \tag{3.11}$$

If $\bar{\bar{\lambda}} = 1$, then the pole to consider is always $z_0^{(IV)}$.

For what concerns the corresponding residues, we obtain

$$\begin{aligned} r(f_2; z_0^{(III)}) &= \frac{\alpha}{(\alpha+1)a^{(IV)}(z_0^{(III)})}\lim_{z\to z_0^{(III)}}\frac{z-z_0^{(III)}}{a^{(III)}(z)} \\ &= \frac{\alpha}{h^{\frac{1}{\alpha}}\lambda\left(1+2\cos(\alpha\pi)(-1)^{\alpha}h\lambda^{\alpha}+(-1)^{2\alpha}h^2\lambda^{2\alpha}\right)} \end{aligned}$$

and

$$\begin{aligned} r(f_2; z_0^{(IV)}) &= \frac{\alpha}{(\alpha+1)a^{(III)}(z_0^{(IV)})}\lim_{z\to z_0^{(IV)}}\frac{z-z_0^{(IV)}}{a^{(IV)}(z)} \\ &= -\frac{ie^{i\alpha\pi}}{2\sin(\alpha\pi)\left(e^{\frac{i(1-\alpha)\pi}{\alpha}}+h^{\frac{1}{\alpha}}\lambda\right)}. \end{aligned}$$

3.2. The final estimates. In order to apply (3.3) it remains to evaluate the terms $\exp\left(-z_0^{(\cdot)}\right)$ and $\exp\left(\sqrt{-z_0^{(\cdot)}}\right)$, where $z_0^{(\cdot)}$ represents one of the four poles to be considered. By (3.5), (3.6), (3.9), (3.10), we immediately have

$$\begin{aligned} \exp(-z_0^{(I)}) &= \frac{e^{-i\alpha\pi}}{h\lambda^{\alpha}}, & \exp(-z_0^{(II)}) &= -e^{i\alpha\pi}, \\ \exp(-z_0^{(III)}) &= (-1)^{\alpha+1}h^{\frac{\alpha+1}{\alpha}}\lambda^{\alpha+1}, & \exp(-z_0^{(IV)}) &= e^{\frac{i(1-\alpha)(\alpha+1)\pi}{\alpha}}. \end{aligned}$$

As for the quantity $\sqrt{-z_0^{(\cdot)}}$, using the relation

$$\sqrt{-iw} = \frac{\sqrt{2}}{2}\,(1-i)\,\sqrt{w}, \quad w \geq 0,$$

we obtain

$$\sqrt{-z_0^{(I)}} = \sqrt{\frac{\alpha}{2}}\,\left(\gamma^-(\lambda) - i\gamma^+(\lambda)\right), \qquad \sqrt{-z_0^{(II)}} = \frac{\sqrt{2}}{2}\,(1-i)\,\sqrt{(1-\alpha)\pi},$$
$$\sqrt{-z_0^{(III)}} = \sqrt{\frac{\alpha+1}{2}}\,\left(\gamma^+(\lambda) + i\gamma^-(\lambda)\right), \quad \sqrt{-z_0^{(IV)}} = \frac{\sqrt{2}}{2}\,(1-i)\,\sqrt{\frac{(1-\alpha)(\alpha+1)}{\alpha}\pi},$$

where

$$\gamma^{\pm}(\lambda) = \sqrt{\sqrt{(\ln(h^{\frac{1}{\alpha}}\lambda))^2 + \pi^2} \pm \ln(h^{\frac{1}{\alpha}}\lambda)}. \tag{3.12}$$

Using the above results and the residues of Section 3.1 in (3.3), we are finally able to write the error estimates for both integrals. For the first one we have

$$e_n^{(1)}(\lambda) \cong \begin{cases} -4\pi\mathfrak{Re}\left(\frac{\alpha e^{-i\alpha\pi} h\lambda^\alpha e^{-\sqrt{2\alpha\bar{n}}\left(\gamma^-(\lambda)+i\gamma^+(\lambda)\right)}}{e^{-2i\alpha\pi}+2h\lambda^\alpha\cos(\alpha\pi)e^{-i\alpha\pi}+h^2\lambda^{2\alpha}}\right) & \text{if } \lambda > \bar{\lambda}, \\ -2\pi\mathfrak{Re}\left(\frac{-ie^{-(1-i)\sqrt{2(1-\alpha)\pi\bar{n}}}}{\sin(\alpha\pi)(1-e^{-i\frac{\pi}{\alpha}}h^{\frac{1}{\alpha}}\lambda)}\right) & \text{if } 1 < \lambda < \bar{\lambda}, \end{cases}$$

($\bar{\lambda}$ defined in (3.8)), and therefore, by taking the modulus,

$$\left|e_n^{(1)}(\lambda)\right| \cong \begin{cases} q_n^{(I)}(\lambda) & \text{if } \lambda > \bar{\lambda}, \\ q_n^{(II)}(\lambda) & \text{if } 1 < \lambda < \bar{\lambda}, \end{cases}$$

where

$$q_n^{(I)}(\lambda) := \frac{4\pi\alpha h\lambda^\alpha e^{-\sqrt{2\alpha\bar{n}}\gamma^-(\lambda)}}{|e^{-2i\alpha\pi} + 2h\lambda^\alpha\cos(\alpha\pi)e^{-i\alpha\pi} + h^2\lambda^{2\alpha}|}, \tag{3.13}$$

$$q_n^{(II)}(\lambda) := \frac{2\pi e^{-\sqrt{2(1-\alpha)\pi\bar{n}}}}{\sin(\alpha\pi)\left|1 - e^{-i\frac{\pi}{\alpha}}h^{\frac{1}{\alpha}}\lambda\right|}. \tag{3.14}$$

We refer to Figure 3.1 for some experiments, where $n = 30$ is fixed and where we consider the behavior of these functions for $\lambda \in \left[1, 10^{16}\right]$ for different values of α and h.

REMARK 3.1. From a theoretical point of view, the estimates (3.13) and (3.14) will not be accurate for λ close to $\bar{\lambda}$ and are incorrect for $\lambda = \bar{\lambda}$. In this situation the poles $z_0^{(I)}$ and $z_0^{(II)}$ are such that the corresponding parabolas $\Gamma_{\mathcal{S}_0^{(I)}}, \Gamma_{\mathcal{S}_0^{(II)}}$ overlap, and then the analysis should take into account the contribution of both poles in the computation of the residues. Nevertheless, as is clearly shown in Figure 3.1(a), 3.1(b), the true error is very well approximated by $q_n^{(\cdot)}(\lambda)$ in the whole interval. In the particular case of $\lambda = \bar{\lambda}$ and $\alpha = 1/2$, we have that $z_0^{(I)} = z_0^{(II)}$, and then formula (3.3) does not work because of a double pole; see the peak in Figure 3.1(c). In order to explore this situation without weighing down the theory in Section 4, we employ some simplifications that come from the evidence that, unlike the estimates, the true error does not explode; see Figure 3.1(d), representing a zoom of

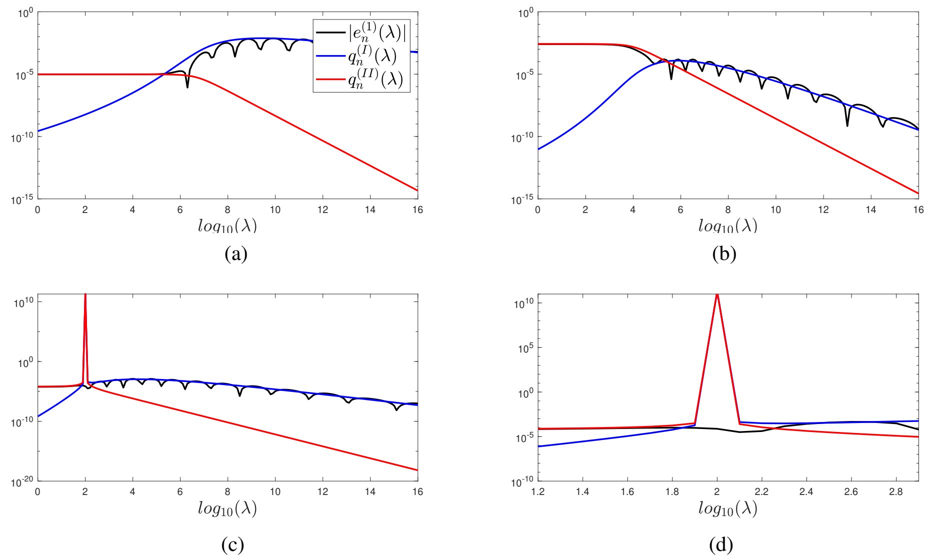

FIG. 3.1. *Behavior of the functions* $\left|e_n^{(1)}(\lambda)\right|$, $q_n^{(I)}(\lambda)$, $q_n^{(II)}(\lambda)$ *for* $\alpha = 0.3$, $h = 10^{-2}$ *(a),* $\alpha = 0.75$, $h = 10^{-3}$ *(b),* $\alpha = 0.5$, $h = 10^{-1}$ *(c). Figure (d) is a zoom of (c) around* $\bar{\lambda}$. *In all cases* $n = 30$.

Figure 3.1(c). The same considerations hold true for the second integral whose final results are given below; see (3.15), (3.16).

For what concerns the error of the second integral, using (3.3) and the previous results, we obtain

$$e_n^{(2)}(\lambda) \cong \begin{cases} 4\pi \mathfrak{Re}\left(\dfrac{\alpha(-1)^\alpha h \lambda^\alpha e^{-\sqrt{2(\alpha+1)\overline{n}}\left(\gamma^+(\lambda)+i\gamma^-(\lambda)\right)}}{1+2\cos(\alpha\pi)(-1)^\alpha h\lambda^\alpha + (-1)^{2\alpha}h^2\lambda^{2\alpha}} \right) & \text{if } 1 \le \lambda < \overline{\overline{\lambda}}, \\ 2\pi \mathfrak{Re}\left(\dfrac{i e^{i\alpha\pi} e^{\frac{i(1-\alpha)(\alpha+1)\pi}{\alpha}}}{\sin(\alpha\pi)\left(e^{\frac{i(1-\alpha)\pi}{\alpha}} + h^{\frac{1}{\alpha}}\lambda\right)} e^{-(1-i)\left(\sqrt{\frac{2(1-\alpha)(\alpha+1)\pi}{\alpha}\overline{n}}\right)} \right) & \text{if } \lambda > \overline{\overline{\lambda}}, \end{cases}$$

where $\overline{\overline{\lambda}}$ is defined in (3.11). Thus we have

$$\left|e_n^{(2)}(\lambda)\right| \cong \begin{cases} q_n^{(III)}(\lambda) & \text{if } 1 \le \lambda < \overline{\overline{\lambda}}, \\ q_n^{(IV)}(\lambda) & \text{if } \lambda > \overline{\overline{\lambda}}, \end{cases}$$

where

$$q_n^{(III)}(\lambda) := \frac{4\pi\alpha h \lambda^\alpha e^{-\sqrt{2(\alpha+1)\overline{n}}\gamma^+(\lambda)}}{|1+2\cos(\alpha\pi)(-1)^\alpha h\lambda^\alpha + (-1)^{2\alpha}h^2\lambda^{2\alpha}|}, \tag{3.15}$$

$$q_n^{(IV)}(\lambda) := \frac{2\pi e^{-\sqrt{\frac{2(1-\alpha)(\alpha+1)\pi}{\alpha}\overline{n}}}}{\sin(\alpha\pi)\left|e^{\frac{i(1-\alpha)\pi}{\alpha}} + h^{\frac{1}{\alpha}}\lambda\right|}. \tag{3.16}$$

We refer to Figure 3.2 for a couple of experiments.

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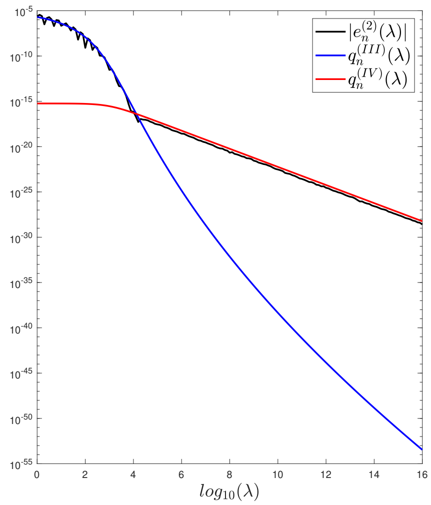
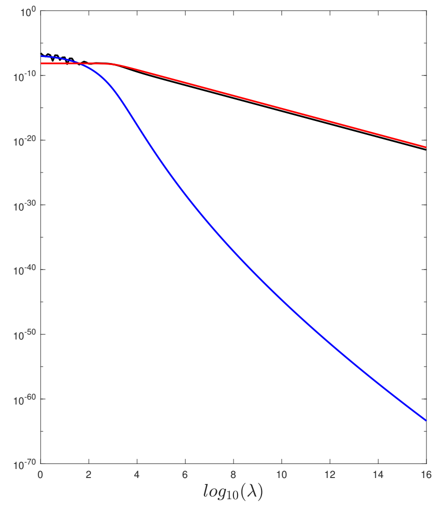


(a)



(b)

FIG. 3.2. *Behavior of the functions* $|e_n^{(2)}(\lambda)|$, $q_n^{(III)}(\lambda)$, $q_n^{(IV)}(\lambda)$ *for* $\alpha = 1/3$, $h = 10^{-1}$ *(a) and* $\alpha = 2/3$, $h = 10^{-2}$ *(b). In both cases* $n = 20$.

4. Error estimates for the operator. By using (1.1), (1.4), and the results of the previous section, the idea now is to estimate the error of the method as follows:

$$\|\mathcal{R}_{h,\alpha}(\mathcal{L}) - R_{k-1,k}(\mathcal{L})\|_{\mathcal{H}\to\mathcal{H}} \cong \frac{\sin(\alpha\pi)}{\alpha\pi}\Bigg(\max\left\{\max_{\lambda\geq\bar{\lambda}} q_n^{(I)}(\lambda),\ \max_{1\leq\lambda\leq\bar{\lambda}} q_n^{(II)}(\lambda)\right\} + \max\left\{\max_{1\leq\lambda\leq\bar{\bar{\lambda}}} q_n^{(III)}(\lambda), \max_{\lambda\geq\bar{\bar{\lambda}}} q_n^{(IV)}(\lambda)\right\}\Bigg).$$

The problem is then reduced to the evaluation of the maxima of the functions $q_n^{(\cdot)}$. Since these functions are not very simple to handle, we are forced to use some further approximations. Note that in the above formula we have included the boundaries $\bar{\lambda}$, $\bar{\bar{\lambda}}$, and thus it does not work for $\alpha = 1/2$; see Figure 3.1(c), 3.1(d). Nevertheless, the used approximation will allow us to solve this issue.

4.1. Approximation of the maxima. We derive approximations of the maxima of the four functions $q_n^{(I)}$, $q_n^{(II)}$, $q_n^{(III)}$, and $q_n^{(IV)}$, defined in (3.13), (3.14), (3.15), and (3.16), respectively.

4.1.1. The function $q_n^{(I)}$. Independently of α and for n large enough, the function reaches a relative maximum at a certain point λ_n (Figure 3.1) and then goes to zero for $\lambda \to \infty$. The problem lies then in the computation of λ_n, and since it grows with n, we simplify (3.13) by observing that

$$\left|\frac{1}{e^{-2i\alpha\pi} + 2h\lambda^\alpha\cos(\alpha\pi)e^{-i\alpha\pi} + h^2\lambda^{2\alpha}}\right| \sim \frac{1}{h^2\lambda^{2\alpha}} \quad \text{for} \quad \lambda \to \infty.$$

Therefore, we can consider the estimate

$$q_n^{(I)}(\lambda) \cong \tilde{q}_n^{(I)}(\lambda) = \frac{4\pi\alpha e^{-\sqrt{2\alpha\bar{n}}\gamma^-(\lambda)}}{h\lambda^\alpha}, \quad \text{for} \quad \lambda \geq \bar{\lambda}. \tag{4.1}$$

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By imposing $\frac{d}{d\lambda}\tilde{q}_n^{(I)}(\lambda)=0$ and defining $s=h^{\frac{1}{\alpha}}\lambda$, after some computation, we obtain

$$\frac{\pi^2}{((\ln s)^2+\pi^2)(\ln s+\sqrt{(\ln s)^2+\pi^2})}=\frac{2\alpha}{\bar{n}}. \tag{4.2}$$

Using $\ln s<\sqrt{(\ln s)^2+\pi^2}$, we have that

$$\frac{\pi^2}{((\ln s)^2+\pi^2)(\ln s+\sqrt{(\ln s)^2+\pi^2})}\geq\frac{\pi^2}{2((\ln s)^2+\pi^2)^{\frac{3}{2}}}.$$

This relation leads to the observation that if $s^\star$ is the solution of (4.2), then there exists a constant d, independent of n, such that

$$(\ln s^*)^3\geq dn. \tag{4.3}$$

Now, by defining

$$\tau(s):=\frac{1}{\sqrt{1+\left(\frac{\pi}{\ln s}\right)^2}},$$

we have

$$\ln s=\tau(s)\sqrt{(\ln s)^2+\pi^2}, \tag{4.4}$$

and hence we can rewrite equation (4.2) as

$$\frac{\pi^2}{(1+\tau(s))((\ln s)^2+\pi^2)^{\frac{3}{2}}}=\frac{2\alpha}{\bar{n}}.$$

By (4.3), $\tau(s^*)\sim 1$, for $n\to\infty$, and therefore

$$s^*\sim\exp\left(\left[\left(\frac{\bar{n}\pi^2}{4\alpha}\right)^{\frac{2}{3}}-\pi^2\right]^{\frac{1}{2}}\right). \tag{4.5}$$

The above relation states that

$$(\ln s^\star)^2+\pi^2\sim\left(\frac{\bar{n}\pi^2}{4\alpha}\right)^{\frac{2}{3}}. \tag{4.6}$$

Let $\lambda^\star=h^{-1/\alpha}s^\star$ be the point of a maximum of $\tilde{q}_n^{(I)}(\lambda)$. Since

$$\gamma^-(\lambda)=\frac{\pi}{\sqrt{\sqrt{(\ln s)^2+\pi^2}+\ln s}},$$

(cf. (3.12)), using (4.4) and (4.6), we have

$$\gamma^-(\lambda^*)\sim\left(\frac{\alpha}{2\bar{n}}\right)^{\frac{1}{6}}\pi^{\frac{2}{3}}.$$

By inserting the above relation and (4.5) in (4.1), we finally obtain

$$\max_{\lambda\geq\bar{\lambda}}q_n^{(I)}(\lambda)\cong\tilde{q}_n^{(I)}(\lambda_n)\sim 4\pi\alpha e^{-c(\bar{n}\alpha^2\pi^2)^{\frac{1}{3}}}=:g_n^{(I)}, \tag{4.7}$$

where

$$c=3\cdot 2^{-\frac{2}{3}}\cong 1.9. \tag{4.8}$$

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4.1.2. The function $q_n^{(II)}$. For what concerns $q_n^{(II)}(\lambda)$, everything depends on the term

$$\left|1 - e^{-i\frac{\pi}{\alpha}} h^{\frac{1}{\alpha}} \lambda\right|^{-1}. \tag{4.9}$$

A simple analysis shows that there is a maximum at

$$h^{\frac{1}{\alpha}} \lambda = \cos \tfrac{\pi}{\alpha}.$$

Therefore for α such that $\cos \frac{\pi}{\alpha} \leq 0$, the function is monotonically decreasing for $\lambda \geq 1$. For α such that $\cos \frac{\pi}{\alpha} > 0$, there is a maximum for $\lambda > 0$ that may be smaller or larger than $\overline{\lambda}$; see (3.8). In any case, however, experimentally one observes that the true error is almost flat at the beginning and then follows the approximation $q_n^{(I)}(\lambda)$ (see Figure 3.1), so that the idea is to consider the approximation

$$\max_{1 \leq \lambda \leq \bar{\lambda}} q_n^{(II)}(\lambda) \cong \frac{2\pi e^{-\sqrt{2(1-\alpha)\pi\bar{n}}}}{\sin(\alpha\pi)} =: g_n^{(II)}, \tag{4.10}$$

which is obtained by neglecting the term (4.9) in (3.14).

4.1.3. The function $q_n^{(III)}$. For n large enough, the function $q_n^{(III)}$ is monotonically decreasing; see Figure 3.2. Thus we have

$$\max_{1 \leq \lambda \leq \bar{\lambda}} q_n^{(III)}(\lambda) = q_n^{(III)}(1) \cong 4\pi\alpha h e^{-\sqrt{2(\alpha+1)\bar{n}}\gamma^{+}(1)}, \tag{4.11}$$

where, as before, we have neglected the term

$$\left|1 + 2\cos(\alpha\pi)(-1)^{\alpha} h\lambda + (-1)^{2\alpha} h^2 \lambda^2\right|^{-1}$$

in (3.15) to prevent the inaccuracy of our formulas whenever the poles $z_0^{(III)}$ and $z_0^{(IV)}$ belong to close parabolas. Experimentally we observe that the accuracy of the approximation (4.11) is poor for small h and α. The reason lies in the fact that the poles $\left\{z_k^{(III)}\right\}$ are too close to each other, and therefore formula (3.3) is not an accurate approximation. Hence, in what follows, we provide an estimate similar to (4.11) that is obtained by removing the dependence on h, that is, by considering the worst case with regard to this parameter. To this end, let

$$\phi(h) := \gamma^{+}(1) = \sqrt{\sqrt{\left(\frac{\ln h}{\alpha}\right)^2 + \pi^2} + \frac{\ln h}{\alpha}};$$

see (3.12). It is easy to show that

$$\phi(h) \sim \frac{\pi}{\sqrt{\frac{2}{\alpha}(-\ln h)}}$$

for $h \to 0$. Now, by using the above approximation in (4.11), we obtain

$$h e^{-\sqrt{2(\alpha+1)\bar{n}}c(h)} \sim e^{\ln h - \sqrt{2(\alpha+1)\bar{n}}\pi\sqrt{\frac{\alpha}{2}}\frac{1}{\sqrt{-\ln h}}} = e^{-y-\sqrt{p}\pi\sqrt{\frac{\alpha}{2}}\frac{1}{\sqrt{y}}}, \tag{4.12}$$

where $y = -\ln h$, $0 < y < +\infty$, for $h < 1$ and $p = 2(\alpha+1)\bar{n}$. Let us consider the function

$$\xi(y) = -y - \sqrt{p}\pi\sqrt{\frac{\alpha}{2}}\frac{1}{\sqrt{y}}.$$

Since $\xi''(y) < 0$ for $y \in (0, +\infty)$, we look for its maximum $\bar{y}$ by solving

$$\frac{d}{dy}\left(-y - \sqrt{p}\sqrt{\frac{\alpha}{2}}\pi\frac{1}{\sqrt{y}}\right) = 0,$$

which leads to

$$\bar{y} = \left(\frac{\sqrt{p}}{2}\sqrt{\frac{\alpha}{2}}\pi\right)^{\frac{2}{3}}.$$

Hence, we have that

$$\xi(\bar{y}) = -cp^{\frac{1}{3}}\left(\frac{\alpha}{2}\right)^{\frac{1}{3}}\pi^{\frac{2}{3}}, \tag{4.13}$$

where c is defined in (4.8). By substituting (4.13) in (4.12) and going back to (4.11), we obtain the new approximation

$$\max_{1\le\lambda\le\bar{\lambda}} q_n^{(III)}(\lambda) \cong 4\pi\alpha e^{-c\left(\alpha(\alpha+1)\pi^2\bar{n}\right)^{\frac{1}{3}}} =: g_n^{(III)}. \tag{4.14}$$

4.1.4. The function $q_n^{(IV)}$. The behavior of the function $q_n^{(IV)}(\lambda)$ is very similar to the one of $q_n^{(II)}(\lambda)$. Therefore we consider the analogous approximation

$$\max_{\lambda\ge\bar{\lambda}} q_n^{(IV)}(\lambda) \cong \frac{2\pi}{\sin(\alpha\pi)} e^{-\sqrt{2\bar{n}\frac{(1-\alpha)(\alpha+1)}{\alpha}\pi}} =: g_n^{(IV)}. \tag{4.15}$$

4.2. Comparison of the bounds. By using (4.7), (4.10), (4.14), (4.15) we now have

$$\begin{aligned}\|\mathcal{R}_{h,\alpha}(\mathcal{L}) - R_{2n-1,2n}(\mathcal{L})\|_{\mathcal{H}\to\mathcal{H}} &\le \frac{\sin(\alpha\pi)}{\alpha\pi}\left(\|e_n^{(1)}(\mathcal{L})\|_{\mathcal{H}\to\mathcal{H}} + \|e_n^{(2)}(\mathcal{L})\|_{\mathcal{H}\to\mathcal{H}}\right)\\ &\cong \frac{\sin(\alpha\pi)}{\alpha\pi}\left(\max\left(g_n^{(I)}, g_n^{(II)}\right) + \max\left(g_n^{(III)}, g_n^{(IV)}\right)\right).\end{aligned} \tag{4.16}$$

The next step is then the comparison of the sequences $g_n^{(\cdot)}$. We start with $g_n^{(I)}$ and $g_n^{(II)}$. Clearly, $g_n^{(I)}$ decays slower asymptotically, and we thus look for an $n^\star$ such that $g_n^{(I)} \ge g_n^{(II)}$ for $n \ge n^\star$. Hence, we have to solve, with respect to n,

$$\frac{2\pi}{\sin(\alpha\pi)} e^{-\sqrt{2\bar{n}(1-\alpha)\pi}} = 4\pi\alpha e^{-c(\bar{n}\alpha^2\pi^2)^{\frac{1}{3}}}.$$

By neglecting the factors before the exponentials and since $\bar{n} = 4n + 2$, we finally obtain

$$n^* \cong \frac{c^6}{2^5}\frac{\alpha^4}{(1-\alpha)^3}\pi - \frac{1}{2}, \tag{4.17}$$

where c is defined in (4.8). By (4.17), we have $n^\star \ge 1$ only for $\alpha \ge \alpha^\star \cong 0.47$, and this is experimentally confirmed. Therefore we have

$$\epsilon_n^{(1)} := \max\left\{g_n^{(I)}, g_n^{(II)}\right\} = \begin{cases} g_n^{(I)} & n \ge n^\star, \\ g_n^{(II)} & 1 \le n < n^\star. \end{cases} \tag{4.18}$$

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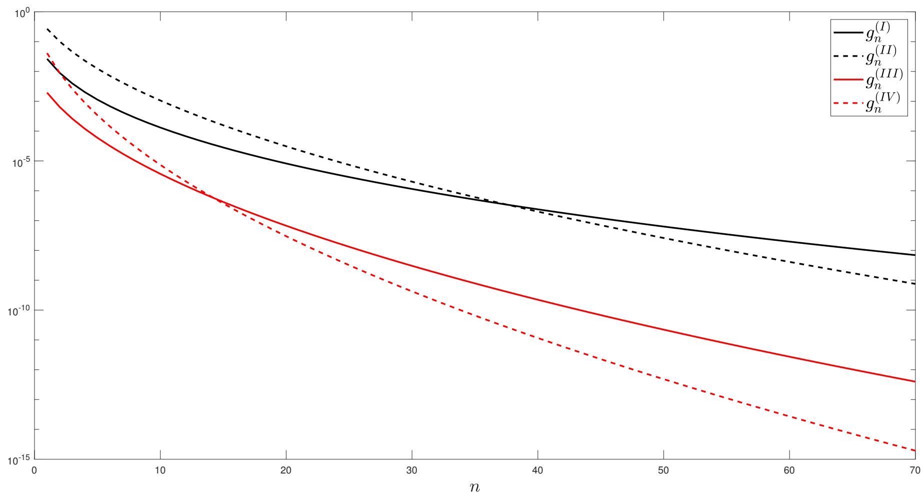

FIG. 4.1. *The behavior of the functions* $g_n^{(\cdot)}$ *for* $\alpha = 0.7$ *and* $h = 10^{-2}$.

The situation is very similar for $g_n^{(III)}$ and $g_n^{(IV)}$ where we have to identify a value $n^{\star\star}$ such that $g_n^{(III)} \geq g_n^{(IV)}$ for $n \geq n^{\star\star}$ by solving

$$4\pi\alpha e^{-c\left((\alpha+1)\bar{n}\alpha\pi^2\right)^{\frac{1}{3}}} = \frac{2\pi}{\sin(\alpha\pi)} e^{-\sqrt{2\bar{n}\frac{(1-\alpha)(\alpha+1)}{2}}\pi}.$$

As before, by neglecting the factors before the exponentials, we find

$$n^{\star\star} \cong \frac{c^6}{2^5}\frac{\alpha^5}{(1-\alpha)^3(1+\alpha)}\pi - \frac{1}{2}. \tag{4.19}$$

Experimentally, we observe that $n^{\star\star} \geq 1$ only for $\alpha \geq \alpha^{\star\star} \cong 0.55$. Moreover, we have that $n^{\star\star} < n^{\star}$ for all α (cf. (4.17) and (4.19)). Finally, we then have

$$\epsilon_n^{(2)} := \max\left\{g_n^{(III)}, g_n^{(IV)}\right\} = \begin{cases} g_n^{(III)} & n \geq n^{\star\star}, \\ g_n^{(IV)} & 1 \leq n < n^{\star\star}. \end{cases} \tag{4.20}$$

In Figure 4.1 we display the sequences $g_n^{(\cdot)}$ for $\alpha = 0.7$ and $h = 10^{-2}$. The analysis just given for $g_n^{(III)}$ and $g_n^{(IV)}$ will be important in the next section. Indeed, for what concerns the error of the method considered so far, we just need to observe (see also Figure 4.1) that

$$\max\left\{g_n^{(III)}, g_n^{(IV)}\right\} \ll \max\left\{g_n^{(I)}, g_n^{(II)}\right\} \quad \forall n,$$

and in particular that the ratio $\epsilon_n^{(2)}/\epsilon_n^{(1)}$ decays exponentially. Thereby, we finally conclude that

$$\begin{aligned} \|\mathcal{R}_{h,\alpha}(\mathcal{L}) - R_{k-1,k}(\mathcal{L})\|_{\mathcal{H}\to\mathcal{H}} &\cong \frac{\sin(\alpha\pi)}{\alpha\pi}\epsilon_n^{(1)} \\ &= \frac{\sin(\alpha\pi)}{\alpha\pi}\begin{cases} 4\pi\alpha e^{-c(\bar{n}\alpha^2\pi^2)^{\frac{1}{3}}} & n \geq n^{\star}, \\ \frac{2\pi e^{-\sqrt{2(1-\alpha)\pi\bar{n}}}}{\sin(\alpha\pi)} & 1 \leq n < n^{\star}. \end{cases} \end{aligned} \tag{4.21}$$

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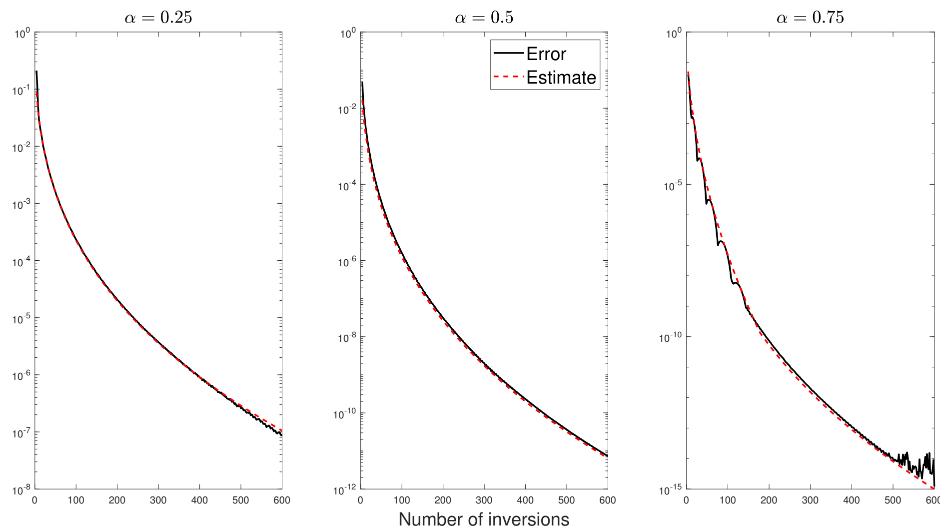

FIG. 4.2. *Error and error estimate* (4.21) *for the computation of* $\mathcal{R}_{h,\alpha}(\mathcal{L})$*, with* $h = 10^{-2}$*. Different values of* α *are considered.*

In order to test the behavior of the method and the accuracy of the error estimate (4.21), we consider the operator

$$\mathcal{L} = \text{diag}\left(10^0, 10^{0.1}, \ldots, 10^{15.9}, 10^{16}\right). \tag{4.22}$$

In Figure 4.2 we display the results for some values of α. Here and below we always consider the spectral norm when working with matrices. While being very simple, the considered operator represents more or less the most difficult situation. Working with Matlab it is also possible to append the constant inf to the diagonal of $\mathcal{L}$. The results are almost indistinguishable.

5. A balanced approach. In this section we present a modification of the Gauss-Laguerre approach that allows us to reduce the number of inversions and hence the computational cost of the method, without loosing accuracy. In fact, since the computation of the first integral requires more points than the second one to achieve the same accuracy, the idea is to find $m \leq n$ such that

$$\max\left(g_n^{(I)}, g_n^{(II)}\right) \cong \max\left(g_m^{(III)}, g_m^{(IV)}\right)$$

and then to consider the approximation

$$\mathcal{R}_{h,\alpha}(\mathcal{L}) \cong \frac{\sin(\alpha\pi)}{\alpha\pi}\left(I_n^{(1)}(\mathcal{L}) + I_m^{(2)}(\mathcal{L})\right).$$

In this setting, we observe that the total number of inversions is $n+m$. By using (4.18), (4.20), and since $n^{\star\star} \leq n^\star$, we have that m can be obtained by imposing

$$\begin{cases} g_n^{(II)} = g_m^{(IV)} & \text{if } 1 \leq n \leq n^{\star\star}, \\ g_n^{(II)} = g_m^{(III)} & \text{if } n^{\star\star} < n \leq n^\star, \\ g_n^{(I)} = g_m^{(III)} & \text{if } n > n^\star. \end{cases}$$

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TABLE 5.1
The values of n and m (5.1) for $\alpha = 0.6$.

n	5	10	15	20	25	50	100
m	2	4	6	8	10	19	38

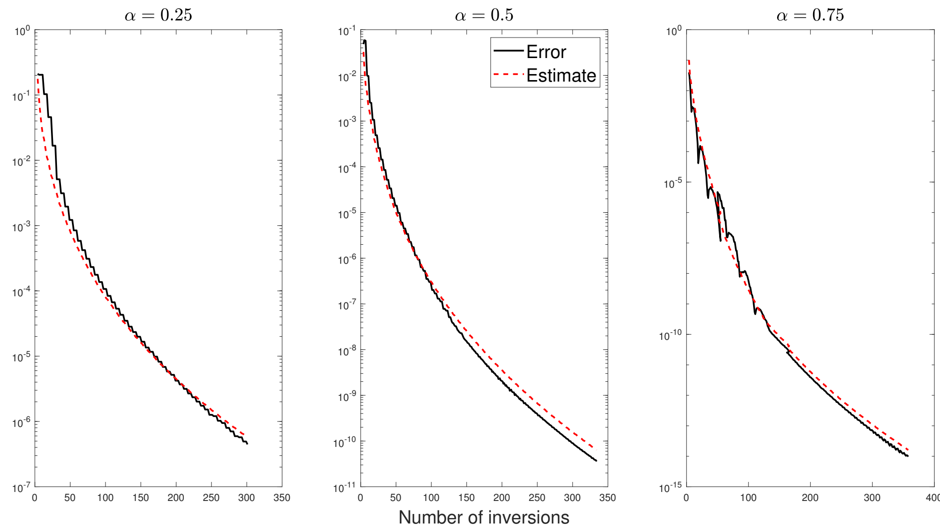

FIG. 5.1. *The error of the balanced approach and the error estimate (5.2) for some values of α and $h = 10^{-2}$.*

After some simple computations, we find that

$$m \cong \begin{cases} \frac{\alpha(2n+1)}{2(\alpha+1)} - \frac{1}{2} & \text{if } 1 \leq n \leq n^{\star\star} \text{ and } n > n^{\star}, \\ \frac{\left(2\sqrt{(2n+1)(1-\alpha)\pi} + \ln(2\alpha\sin(\alpha\pi))\right)^3}{27(\alpha+1)\alpha\pi^2} - \frac{1}{2} & \text{if } n^{\star\star} < n \leq n^{\star}. \end{cases} \tag{5.1}$$

An example is reported in Table 5.1, where m is defined by using the floor operator applied to (5.1). The error is then finally estimated by (cf. (4.16)):

$$\|\mathcal{R}_{h,\alpha}(\mathcal{L}) - R_{n+m-1,n+m}(\mathcal{L})\|_{\mathcal{H}\to\mathcal{H}} \cong 2\frac{\sin(\alpha\pi)}{\alpha\pi}\max\left(g_n^{(I)}, g_n^{(II)}\right). \tag{5.2}$$

In Figure 5.1, working with the operator (4.22), we plot the error and the error estimate (5.2) for some values of α and $h = 10^{-2}$. In order to have an expression of the estimates that depends on the total number of inversions $q = n + m$, by (5.1), we observe that for $n > n^{\star}$

$$m \cong \frac{\alpha}{\alpha+1}n,$$

and therefore

$$q = \frac{2\alpha+1}{\alpha+1}n.$$

By using (4.7), (4.8), and (5.2) we then obtain

$$\|\mathcal{R}_{h,\alpha}(\mathcal{L}) - R_{q-1,q}(\mathcal{L})\|_{\mathcal{H}\to\mathcal{H}} \cong 8\sin(\alpha\pi)e^{-3\left(q\frac{\alpha+1}{2\alpha+1}\alpha^2\pi^2\right)^{\frac{1}{3}}}.$$

Note that without balancing, that is for $q = 2n$, again by (4.7) we have

$$\|\mathcal{R}_{h,\alpha}(\mathcal{L}) - R_{q-1,q}(\mathcal{L})\|_{\mathcal{H}\to\mathcal{H}} \cong 4\sin(\alpha\pi)e^{-3\left(\frac{1}{2}q\alpha^2\pi^2\right)^{\frac{1}{3}}}.$$

By comparing the two estimates we observe that, asymptotically, the speedup is then provided by the constant

$$\frac{4}{3} < \frac{2\alpha+2}{2\alpha+1} < 2.$$

6. A truncated approach. In this section we present an additional approach, already used in [4], to further reduce the total number of inversions without loss of accuracy. In particular, since the weights of the Gauss-Laguerre rule decay exponentially (see, e.g., [13]), the idea is to find $k_n < n$ and $k_m < m$ such that we can suitably neglect the tails of the quadrature formulas $I_n^{(1)}(\mathcal{L})$ and $I_m^{(2)}(\mathcal{L})$ and therefore consider the approximation

$$\mathcal{R}_{h,\alpha}(\mathcal{L}) \cong \frac{\sin(\alpha\pi)}{\alpha\pi}\left(I_{k_n}^{(1)}(\mathcal{L}) + I_{k_m}^{(2)}(\mathcal{L})\right), \tag{6.1}$$

where

$$I_{k_n}^{(1)}(\lambda) := \sum_{j=1}^{k_n} w_j^{(n)} f_1(x_j^{(n)}) \quad \text{and} \quad I_{k_m}^{(2)}(\lambda) := \sum_{j=1}^{k_m} w_j^{(m)} f_2(x_j^{(m)}).$$

In this setting, the total number of inversions is $k_n + k_m$. We start the analysis by recalling that the sequences of error approximations of the two integrals, denoted by $\{\epsilon_n^{(1)}\}_{n\geq 1}$ and $\{\epsilon_m^{(2)}\}_{m\geq 1}$ (see (4.18), (4.20)), are such that $\epsilon_n^{(1)} \cong \epsilon_m^{(2)}$, because of the balancing introduced in the previous section. Remembering that for the functions f_1 and f_2 (see (2.2), (2.3)) one has that $0 \leq f_i(x) \leq K_i$, $i = 1, 2$, uniformly with respect to $1 \leq \lambda < +\infty$ and with K_i as in (2.4), we now have

$$\int_0^{+\infty} e^{-x} f_i(x)dx \leq K_i \int_0^{+\infty} e^{-x}dx, \quad i = 1, 2.$$

At this point, let $s_n^{(1)}$ and $s_m^{(2)}$ be, respectively, the solutions of

$$K_1 \int_{s_n^{(1)}}^{+\infty} e^{-x}dx = \epsilon_n^{(1)} \quad \text{and} \quad K_2 \int_{s_m^{(2)}}^{+\infty} e^{-x}dx = \epsilon_m^{(2)}.$$

From the above equations,

$$s_n^{(1)} = -\ln\left(\frac{\epsilon_n^{(1)}}{K_1}\right) \quad \text{and} \quad s_m^{(2)} = -\ln\left(\frac{\epsilon_m^{(2)}}{K_2}\right). \tag{6.2}$$

Then, for the first integral we consider the truncated rule $I_{k_n}^{(1)}$, where k_n is the smallest integer such that $x_j^{(n)} \geq s_n^{(1)}$ for all $j \geq k_n$. We observe that

$$\begin{aligned}\left\|I^{(1)}(\mathcal{L}) - I_{k_n}^{(1)}(\mathcal{L})\right\|_{\mathcal{H}\to\mathcal{H}} &= \left\|I^{(1)}(\mathcal{L}) - I_n^{(1)}(\mathcal{L}) + \sum_{j=k_n+1}^{n} w_j^{(n)} f_1(x_j^{(n)})\right\|_{\mathcal{H}\to\mathcal{H}} \\ &\leq \epsilon_n^{(1)} + \sum_{j=k_n+1}^{n} w_j^{(n)} f_1(x_j^{(n)}) \leq \epsilon_n^{(1)} + K_1 \sum_{j=k_n+1}^{n} w_j^{(n)}.\end{aligned}$$

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Now, by using the bound (see [13])

$$w_j^{(n)} \le C(x_j^{(n)} - x_{j-1}^{(n)})e^{-x_j^{(n)}},$$

where C is a constant independent of n and close to 1, we have (see (6.2))

$$\sum_{j=k_n+1}^{n} w_j^{(n)} \le C \sum_{j=k_n+1}^{n} \left(x_j^{(n)} - x_{j-1}^{(n)}\right) e^{-x_j^{(n)}} \le C \int_{x_{k_n}^{(n)}}^{+\infty} e^{-x} dx$$
$$= Ce^{-x_{k_n}^{(n)}} \le Ce^{-s_n^{(1)}} = C\epsilon_n^{(1)},$$

and finally

$$\left\| I^{(1)}(\mathcal{L}) - I_{k_n}^{(1)}(\mathcal{L}) \right\|_{\mathcal{H}\to\mathcal{H}} \le (1+C)\epsilon_n^{(1)} \cong 2\epsilon_n^{(1)}. \tag{6.3}$$

As for the second integral, by following the same arguments, we obtain

$$\left\| I^{(2)}(\mathcal{L}) - I_{k_m}^{(2)}(\mathcal{L}) \right\|_{\mathcal{H}\to\mathcal{H}} \le (1+C)\epsilon_m^{(2)} \cong 2\epsilon_m^{(2)}, \tag{6.4}$$

where k_m is the smallest integer such that $x_j^{(m)} \ge s_m^{(2)}$ for all $j \ge k_m$. It is interesting to observe that it is also possible to derive an analytical approximate expression for k_n and k_m that allows us to understand the behavior of the error with respect to $k_n + k_m$. The analysis makes use of the relation

$$x_j^{(n)} = c_j \frac{j^2\pi^2}{4n}\left(1 + \mathcal{O}\left(\frac{1}{n^2}\right)\right), \tag{6.5}$$

with $1 < c_j < \left(1+\frac{1}{j}\right)^2$, given in [4, Prop. 6.1]. We start with the computation of k_n for $1 \le n \le n^*$. In this case the error $\epsilon_n^{(1)}$ is given by $g_n^{(II)}$ (see (4.10), (4.18)), and therefore

$$s_n^{(1)} = -\ln\left(\frac{g_n^{(II)}}{K_1}\right) = -\ln\left(\frac{2\pi}{\sin(\alpha\pi)}\right) + \sqrt{2\bar{n}(1-\alpha)\pi},$$

(since $K_1 = 1$). By neglecting the term $\ln\left(\frac{2\pi}{\sin(\alpha\pi)}\right)$ and since $\bar{n} = 4n+2$, we obtain

$$s_n^{(1)} \cong \sqrt{8n(1-\alpha)\pi}.$$

Recalling that k_n is such that $x_{k_n}^{(n)} \ge s_n^{(1)}$ and using the relation (6.5), we try to solve, with respect to j,

$$\sqrt{8n(1-\alpha)\pi} = c_j \frac{j^2\pi^2}{4n}.$$

By using $c_j \cong 1$ and the floor operator $\lfloor\cdot\rfloor$, we have that

$$j_n := \left\lfloor 2(1-\alpha)^{\frac{1}{4}} \left(\frac{2n}{\pi}\right)^{\frac{3}{4}} \right\rfloor \tag{6.6}$$

is a good approximation of k_n. Note that $j_n \le n$ for all n and α. From the above expression we can compute n in terms of j_n, that is,

$$n \cong \pi \left[\frac{j_n^4}{2^7(1-\alpha)}\right]^{\frac{1}{3}} \quad \text{for} \quad 1 \le n \le n^\star. \tag{6.7}$$

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TABLE 6.1
The values of m, k_n, j_n, k_m, and j_m with respect to n in the case of $\alpha = 0.75$.

$\boldsymbol{n}$	5	10	15	20	25	50	100
$\boldsymbol{m}$	2	4	7	9	11	16	46
$\boldsymbol{k_n(j_n)}$	3(2)	5(4)	7(6)	9(8)	10(10)	18(18)	30(30)
$\boldsymbol{k_m(j_m)}$	2(2)	4(4)	5(6)	6(6)	7(8)	11(10)	21(22)

Following the same steps, for $n > n^*$, we obtain

$$j_n := \left\lfloor 2\sqrt{3}\left(\frac{\alpha n^2}{\pi^2}\right)^{\frac{1}{3}}\right\rfloor \cong k_n, \tag{6.8}$$

from which

$$n \cong \frac{\pi}{\sqrt{\alpha}}\left[\frac{j_n}{2\sqrt{3}}\right]^{\frac{3}{2}} \quad \text{for } n > n^*. \tag{6.9}$$

Finally, by using the approximations (6.7) and (6.9) in (4.18), we obtain

$$\epsilon_n^{(1)} \cong \begin{cases} 4\pi\alpha e^{-3^{3/4}2^{-1/2}\alpha^{1/2}\pi j_n^{1/2}} & \text{if } n > n^\star, \\ \frac{2\pi}{\sin(\alpha\pi)} e^{-2^{1/3}(1-\alpha)^{1/3}\pi j_n^{2/3}} & \text{if } 1 \le n \le n^\star. \end{cases} \tag{6.10}$$

For the second integral the analysis is the same. Remember that $K_2 = \frac{\alpha}{\alpha+1}h^{-1/\alpha}$. Then, for $1 \le m \le m^{\star\star}$, we find

$$j_m := \left\lfloor\left\{\frac{4m}{\pi^2}\left[\ln\left(\frac{\alpha}{\alpha+1}h^{-\frac{1}{\alpha}}\right) + \sqrt{\frac{8m(1-\alpha)(\alpha+1)\pi}{\alpha}}\right]\right\}^{\frac{1}{2}}\right\rfloor \cong k_m, \tag{6.11}$$

and for $m \ge m^{**}$, we have that

$$j_m := \left\lfloor\left\{\frac{4m}{\pi^2}\left[\ln\left(\frac{\alpha}{\alpha+1}h^{-\frac{1}{\alpha}}\right) + 3\left((\alpha+1)\alpha\pi^2 m\right)^{\frac{1}{3}}\right]\right\}^{\frac{1}{2}}\right\rfloor \cong k_m. \tag{6.12}$$

At this point we are able to write down the final error estimates. From (6.3), (6.4), (6.10), and since $\epsilon_n^{(1)} \cong \epsilon_m^{(2)}$, we obtain

$$\begin{aligned} \left\|\mathcal{R}_{h,\alpha}(\mathcal{L}) - R_{q-1,q}(\mathcal{L})\right\|_{\mathcal{H}\to\mathcal{H}} & \\ \le \frac{\sin(\alpha\pi)}{\alpha\pi}&\left(\left\|I^{(1)}(\mathcal{L}) - I^{(1)}_{j_n}(\mathcal{L})\right\|_{\mathcal{H}\to\mathcal{H}} + \left\|I^{(2)}(\mathcal{L}) - I^{(2)}_{j_m}(\mathcal{L})\right\|_{\mathcal{H}\to\mathcal{H}}\right) \\ \cong 4\frac{\sin(\alpha\pi)}{\alpha\pi}&\epsilon_n^{(1)} \\ \cong 4\frac{\sin(\alpha\pi)}{\alpha\pi}&\begin{cases} 4\pi\alpha e^{-c\pi 2^{1/6}3^{-1/4}\alpha^{1/2}j_n^{1/2}} & \text{if } n > n^\star, \\ \frac{2\pi}{\sin(\alpha\pi)} e^{-3^{3/4}2^{-1/2}\alpha^{1/2}\pi j_n^{1/2}} & \text{if } 1 \le n \le n^\star, \end{cases} \end{aligned} \tag{6.13}$$

where $q = j_n + j_m$. In Table 6.1 we list the values of m, k_n, k_m, together with the theoretical approximations j_n and j_m, with respect to n, for the case of $\alpha = 0.75$. The approximations provided by j_n and j_m are fairly accurate. In order to have an asymptotic expression for the estimate (6.13) that depends on the total number of inversions q, we first consider for (6.12) the approximation

$$j_m \cong [12\pi^{-\frac{4}{3}}(\alpha+1)^{\frac{1}{3}}\alpha^{\frac{1}{3}}m^{\frac{4}{3}}]^{\frac{1}{2}} \quad \text{for } m > m^\star,$$

and hence

$$m \cong \frac{\pi}{2^{3/2}3^{3/4}(\alpha+1)^{1/4}\alpha^{1/4}} j_m^{\frac{3}{2}}.$$

By using the above approximation in $g_m^{(III)}$ (see (4.14)), we obtain

$$g_m^{(III)} \cong 4\pi\alpha e^{-3^{3/4}2^{1/2}\alpha^{1/4}(\alpha+1)^{1/4}\pi j_m^{1/2}}.$$

Moreover, since $\epsilon_n^{(1)} \cong \epsilon_m^{(2)}$, we have that

$$3^{\frac{3}{4}}2^{-\frac{1}{2}}\pi\alpha^{\frac{1}{2}}j_n^{\frac{1}{2}} \cong 3^{\frac{3}{4}}2^{-\frac{1}{2}}\pi\alpha^{\frac{1}{4}}(\alpha+1)^{\frac{1}{4}}j_m^{\frac{1}{2}},$$

and therefore

$$j_n + j_m \cong \left[1 + \left(\frac{\alpha}{\alpha+1}\right)^{\frac{1}{2}}\right] j_n.$$

Then, by (6.13), we finally arrive at the asymptotic estimate

$$\begin{aligned} &\|\mathcal{R}_{h,\alpha}(\mathcal{L}) - R_{q-1,q}(\mathcal{L})\|_{\mathcal{H}\to\mathcal{H}} \\ &\qquad \cong 16\sin(\alpha\pi)\exp\left(-3^{\frac{3}{4}}2^{-\frac{1}{2}}\pi\alpha^{\frac{1}{2}}\left[1+\left(\frac{\alpha}{\alpha+1}\right)^{\frac{1}{2}}\right]^{-\frac{1}{2}} q^{\frac{1}{2}}\right). \end{aligned} \tag{6.14}$$

As an example of the remarkable improvements of the balanced and truncated approach, working with operator (4.22), in Figure 6.1 we display the error and the error estimate (6.13), while in Figure 6.2 we compare the three approaches developed in this work, for different values of α and $h = 10^{-2}$. Finally, in Algorithm 1 we summarize the steps necessary to implement the method.

Algorithm 1 Balanced and truncated Gauss-Laguerre method.

Input: $\alpha, h, \mathcal{L}$
  evaluate $n^\star$, $n^{\star\star}$ using (4.17), (4.19)
  for $n = 1, \dots$ **do**
    evaluate m using (5.1)
    compute $w_j^{(n)}$, $x_j^{(n)}$ and $w_j^{(m)}$, $x_j^{(m)}$
    evaluate j_n ((6.6), (6.8)) and j_m ((6.11), (6.12))
    calculate the approximation (6.1)
  end for

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7. Conclusions. In this work we have described an efficient method for the computation of the resolvent of the fractional powers of a self-adjoint positive operator in the continuous setting of a generic Hilbert space. The use of the Gauss-Laguerre rule, with the improvements

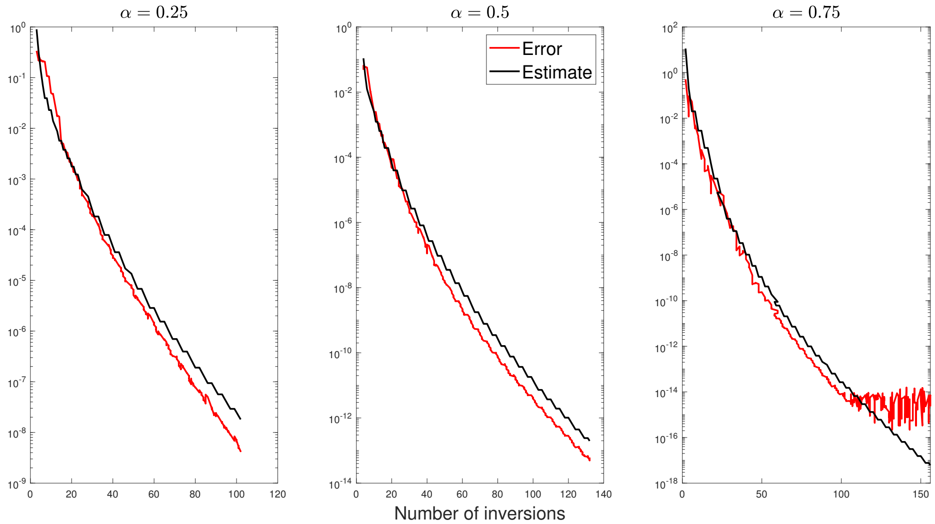

FIG. 6.1. *The error of the truncated approach and the error estimate* (6.13) *for some values of* α *and* $h = 10^{-2}$.

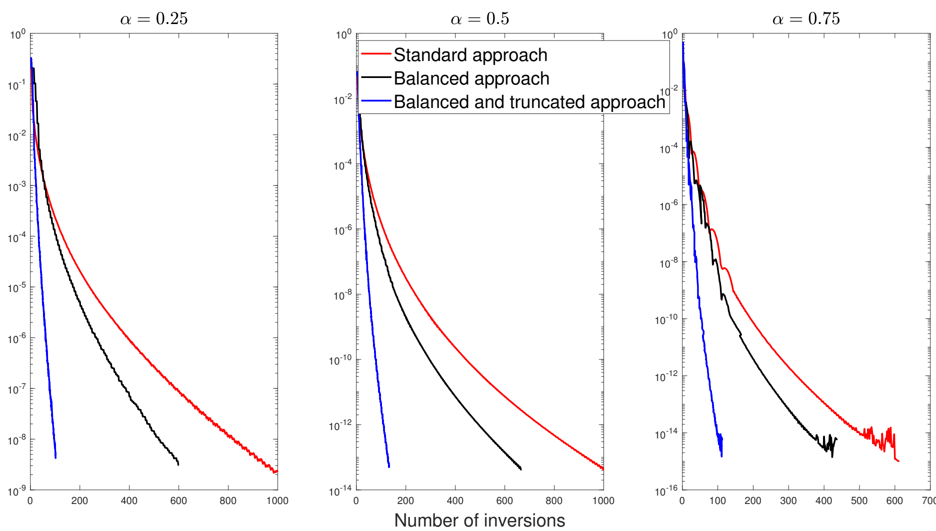

FIG. 6.2. *Comparisons between the errors of the three approaches (standard, balanced, balanced, and truncated) for different values of* α *and* $h = 10^{-2}$.

developed in Section 5 and 6, leads to a method whose rate of convergence is the same as in the scalar case of the type $\exp(-\text{const} \cdot q^{1/2})$, where q represents the number of inversions (cf. the definitions of $q_n^{(\cdot)}(\lambda)$ in Section 3.2 and formula (6.14)). Moreover, we have provided accurate error estimates even if we have been forced to adopt approximations only justified by experimental evidences in Section 4.1. We also remark that the final algorithm (Algorithm 1) does not require any additional parameters. It only needs the code for the computation of the Gauss-Laguerre nodes and weights, for which we have employed the Matlab function lagpts.m from chebfun; see [16].

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