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On approximate inverse of Hermite and Laguerre collocation differentiation matrices and new collocation schemes in unbounded domains

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ABSTRACT

In this paper, we provide an explicit, stable and fast means to compute the approximate inverse of Hermite/Laguerre collocation differentiation matrices, and also the approximate inverse of the Hermite/Laguerre collocation matrices of a second-order differential operator. The latter offers optimal preconditioners for developing well-conditioned Hermite/Laguerre collocation schemes. We apply the new approaches to various partial differential equations in unbounded domains and demonstrate the advantages over the usual collocation methods.

1. Introduction

The spectral methods are capable of providing very accurate simulation results with a relatively smaller number of degree of freedoms when compared with lower-order methods, so they are playing an ever increasingly important role in various computations related to a wide range of applications (see, e.g., [1–6] and the references therein). Among several versions of spectral algorithms, the spectral collocation method is implemented straightforwardly in the physical space, and performs differentiation on a set of preassigned collocation points, where the equation under consideration is required to be satisfied, so it has remarkable advantages in dealing with variable coefficient and/or nonlinear problems. However, the practitioners are oftentimes plagued with ill-conditioning of the resulted linear systems.

It is known that the construction of suitable preconditioners is an effective means to circumvent this barrier. To date, considerable progress has been made in preconditioning spectral methods on finite domains. The successful attempts particularly include preconditioning usual collocation schemes by low-order finite difference or finite elements (see, e.g., [7–13]); and preconditioning differentiation by integration (see, e.g., [14–23]). We highlight that Costabile and Longo [24] proposed the Birkhoff–Lagrange collocation methods using some interpolating basis polynomials associated with a suitable Birkhoff interpolation problem (cf. [25]) for boundary value problems (BVPs). Remarkably, Wang et al. [22] showed that

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such an approach led to well-conditioned collocation schemes and offered optimal preconditioners for usual collocation schemes. We refer to e.g., [26–31] for recent followups and extensions of the Birkhoff collocation notion. It is important to remark that the method in [22,24] can be thought of as the collocation analogue of the spectral-Galerkin method based on compact combinations of orthogonal polynomials [32,33] in the sense that in both cases, the matrix corresponding to the highest derivative is diagonal. This turns out to be the key to the success of producing well-conditioned linear systems. We also mention the recent interest in constructing Fourier-like basis that can inherit the merit of Fourier basis, leading to diagonal mass and stiffness matrices for any linear differential operator with constant coefficients (cf. [34–36]), and the recent advances in developing efficient spectral algorithms [37–39].

The main purpose of this paper is to develop well-conditioned Laguerre and Hermite Birkhoff-collocation methods in unbounded domains having the same advantages as their counterparts in bounded domains [22,24]. However, a significant difficulty is that in latter case, the magnitude of the smallest eigenvalues of the spectral collocation-differentiation matrices behave like a constant (cf. [40,41]), but in the Laguerre and Hermite cases, it decays with respect to N (cf. [42] and also see Fig. 2.1–2.2). As a result, the preconditioning differentiation by integration via Birkhoff interpolation in [22,24] fails to produce well-conditioned systems (see (2.27), (2.28) and (2.35)). In light of [28], we take the approach of inverting the elliptic operator: $\mathcal{L}_\nu[u] = u'' - \nu^2 u$ in a finite dimensional approximation space explicitly. This leads to a new basis that generates the approximate inverse of the collocation matrix corresponding to this operator, so as to be able to nearly optimally precondition the collocation system. In particular, for some special value $\nu = 1/2$, it leads to exact inverse (see (3.37) and with much simpler explicit formula for calculating the basis). As a by-product, we further the study of eigenvalues of Laguerre and Hermite differentiation matrices in [42] through the notion of Birkhoff interpolation in unbounded domains. It is expected that the collocation methods and preconditioning techniques can provide viable tools for practical models in unbounded domains (see, e.g., [43–45]).

The rest of the paper is organized as follows. In Section 2, we provide an explicit means to calculate the approximate inverse of the Hermite and Laguerre differentiation matrices which motivates the studies in the forthcoming sections. In Section 3, we construct the new basis for both Laguerre and Hermite cases and introduce efficient algorithms for the related calculations. In Section 4, we consider the applications of the new approach to various problems in unbounded domains and supply with ample numerical comparison and results to show the high accuracy and efficiency of the proposed approaches.

2. Collocation differentiation matrices and their approximate inverse

In this section, we further the study of eigenvalues and conditioning of the collocation differentiation matrices associated with Hermite and Laguerre functions in [42]. We construct their approximate inverse through integrating the interpolating basis functions to motivate the studies in the subsequent sections. We also review some relevant properties of Hermite and Laguerre functions to be used throughout the paper.

2.1. Hermite functions and Hermite collocation differentiation matrices

Let $H_k(x), x \in \mathbb{R} := (-\infty, \infty)$ be the Hermite polynomial of degree k, satisfying

$$\int_{\mathbb{R}} H_k(x)H_l(x)e^{-x^2}\mathrm{d}x = \sqrt{\pi}2^l l!\,\delta_{kl}, \tag{2.1}$$

where δ_{kl} is the Kronecker function. It is odd (resp. even) for k odd (resp. even), i.e.,

$$H_k(-x) = (-1)^k H_k(x). \tag{2.2}$$

Define the corresponding Hermite functions as

$$\widehat{H}_k(x) = \frac{1}{\pi^{1/4}\sqrt{2^k k!}} e^{-x^2/2} H_k(x), \quad k \geq 0, \tag{2.3}$$

which are orthonormal in $L^2(\mathbb{R})$. By [6, (7.75)], we have

$$\widehat{H}_k'(x) = \sqrt{\frac{k}{2}}\,\widehat{H}_{k-1}(x) - \sqrt{\frac{k+1}{2}}\,\widehat{H}_{k+1}(x), \quad k \geq 1. \tag{2.4}$$

Let $\mathcal{P}_N(\mathbb{R})$ be the set of all polynomials of degree at most N on $\mathbb{R}$, and denote

$$\widehat{\mathcal{P}}_N(\mathbb{R}) = \mathrm{span}\big\{\widehat{H}_0(x), \widehat{H}_1(x), \ldots, \widehat{H}_N(x)\big\} = \big\{u = e^{-x^2/2}v \,:\, v \in \mathcal{P}_N(\mathbb{R})\big\}. \tag{2.5}$$

Recall the Hermite–Gauss quadrature rule with the nodes $\{x_j\}_{j=0}^N$ being all zeros of $H_{N+1}(x)$, and the corresponding weights given by

$$\omega_j = \frac{1}{(N+1)\widehat{H}_N^2(x_j)}, \quad 0 \leq j \leq N.$$

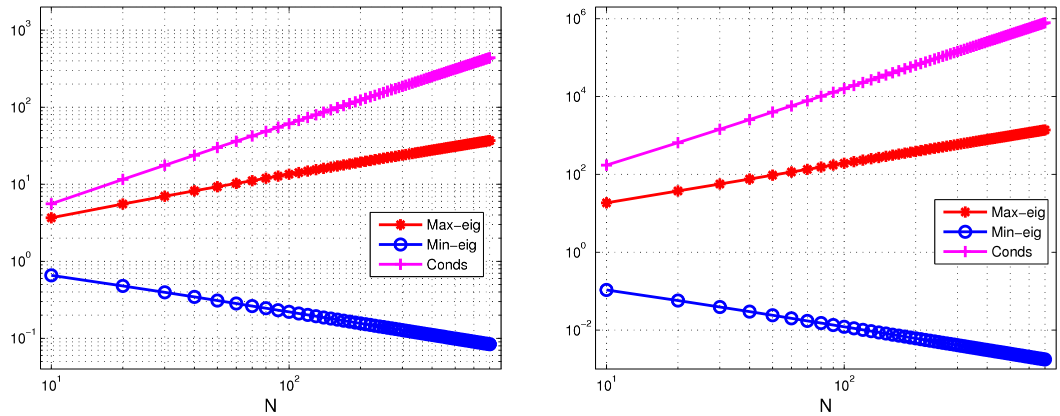

Fig. 2.1. The modulus of the largest, smallest eigenvalues and condition numbers in log–log scale. Left: $\boldsymbol{D}^{(1)}$; Right: $\boldsymbol{D}^{(2)}$.

Then we have the exactness of quadrature (cf. [6, Ch. 7]):

$$\int_{\mathbb{R}} p(x)q(x)\mathrm{d}x = \sum_{j=0}^{N} p(x_j)q(x_j)\omega_j, \tag{2.6}$$

where $p \in \widehat{\mathcal{P}}_L(\mathbb{R})$ and $q \in \widehat{\mathcal{P}}_M(\mathbb{R})$ with $L + M \leq 2N + 1$.

Let $\{l_j\}$ be the Lagrange interpolating basis polynomials associated with the Hermite–Gauss points $\{x_j\}_{j=0}^N$, and $\{h_j\}$ be the corresponding interpolating basis associated with the Hermite functions, that is,

$$h_j(x) = e^{(x_j^2-x^2)/2}\, l_j(x), \quad l_j \in \mathcal{P}_N(\mathbb{R}), \quad l_j(x_i) = \delta_{ij}, \quad 0 \leq j \leq N. \tag{2.7}$$

Moreover, we find from (2.6) and (2.7) that

$$h_j(x) = \sum_{k=0}^{N} \omega_j \widehat{H}_k(x_j)\, \widehat{H}_k(x) \in \widehat{\mathcal{P}}_N(\mathbb{R}), \quad 0 \leq j \leq N. \tag{2.8}$$

Indeed, as $h_j \in \widehat{\mathcal{P}}_N(\mathbb{R})$, we can expand it as

$$h_j(x) = \sum_{k=0}^{N} \alpha_k^j\, \widehat{H}_k(x), \quad 0 \leq j \leq N,$$

so by (2.1), (2.3), (2.6) and (2.7),

$$\alpha_k^j = \int_{\mathbb{R}} h_j(x)\widehat{H}_k(x)\,\mathrm{d}x = \widehat{H}_k(x_j)\omega_j, \quad 0 \leq k, j \leq N.$$

Define the mth-order differentiation matrix: $\boldsymbol{D}^{(m)} = \big(d_{ij}^{(m)} := h_j^{(m)}(x_i)\big)_{0\leq i,j\leq N}$ (see, e.g., [6] for their evaluation). Weideman [42, Thm 3] showed that the eigenvalues of $\boldsymbol{D}^{(1)}$ are all distinct, purely imaginary, and given by $\lambda_j = \mathrm{i}x_j$, where x_j are the roots of $H_{N+1}(x)$. It was also proven in [42, Thm 4] that the eigenvalues of $\boldsymbol{D}^{(2)}$ are real, negative and distinct, and given by $\lambda_j = -\nu_j^2$, where the ν_j are $[(N+1)/2]$ positive roots of $H_{N+1}(x)$, together with the interlacing $[(N+2)/2]$ positive roots of $H'_{N+1}(x) - xH_{N+1}(x)$. As a result, we have that for $\boldsymbol{D}^{(1)}$,

$$\min_j |\lambda_j| = O\big(1/\sqrt{N}\big), \quad \max_j |\lambda_j| = O(\sqrt{N}), \quad \mathrm{Cond}(\boldsymbol{D}^{(1)}) = O(N), \tag{2.9}$$

and for $\boldsymbol{D}^{(2)}$,

$$\min_j |\lambda_j| = O\big(N^{-1}\big), \quad \max_j |\lambda_j| = O(N), \quad \mathrm{Cond}(\boldsymbol{D}^{(2)}) = O(N^2). \tag{2.10}$$

The plots in Fig. 2.1 indeed agree with these predictions.

It should be pointed out the behaviours (2.9) and (2.10) are very different from those of the Legendre and Chebyshev cases, where the magnitude of the smallest eigenvalues behaves likes a constant, while that of the largest eigenvalues grows like $O(N^2)$ and $O(N^4)$ for the first-order and second-order differentiation matrices, respectively. As shown in [22], the property $\min_j |\lambda_j| = O(1)$ is the key to the success of the design of well-conditioned Legendre and Chebyshev collocation schemes by using integration preconditioning through explicitly and stably evaluating the inverse of the highest order differentiation matrix using the Birkhoff interpolation. However, this explicit approach cannot be directly applied to this setting largely due to that for $u \in \widehat{\mathcal{P}}_N(\mathbb{R})$, $u' \notin \widehat{\mathcal{P}}_N(\mathbb{R})$. Consequently, we resort to the method in [26] to find an "approximate" inverse. For this purpose, we introduce

$$p_j^{(1)}(x) = \int_{-\infty}^{x} h_j(t)\,dt, \quad p_j^{(2)}(x) = \frac{1}{2}\int_{-\infty}^{x}(x-t)h_j(t)\,dt + \frac{1}{2}\int_{x}^{\infty}(t-x)h_j(t)\,dt, \tag{2.11}$$

which can be computed stably by using (2.8) and the three-term recurrence formula of Hermite functions (cf. [6, (7.73)]).

Proposition 2.1. *Let $\{p_j^{(1)}, p_j^{(2)}\}$ be defined as in (2.11), and define the matrices $\boldsymbol{P}^{(1)}, \boldsymbol{P}^{(2)}$ with the ijth entries: $p_j^{(1)}(x_i), p_j^{(2)}(x_i)$, respectively. Then we have*

$$\boldsymbol{P}^{(1)}\boldsymbol{D}^{(1)} \approx \boldsymbol{I}_{N+1}, \quad \boldsymbol{P}^{(2)}\boldsymbol{D}^{(2)} \approx \boldsymbol{I}_{N+1}, \tag{2.12}$$

where $\boldsymbol{I}_{N+1}$ is an identity matrix.

Proof. Consider the approximation of $h_j'(x)$ (note: $h_j' \notin \widehat{\mathcal{P}}_N(\mathbb{R})$) by its Hermite–Gauss interpolation:

$$h_j'(x) \approx \sum_{k=0}^{N} h_j'(x_k)h_k(x), \quad \text{so} \quad h_j(x) \approx \sum_{k=0}^{N} h_j'(x_k)\int_{-\infty}^{x} h_k(t)dt. \tag{2.13}$$

Taking $x = x_i$, we obtain

$$\delta_{ij} \approx \sum_{k=0}^{N} p_k^{(1)}(x_i)\, d_{kj}^{(1)}, \quad \text{so} \quad \boldsymbol{I}_{N+1} \approx \boldsymbol{P}^{(1)}\boldsymbol{D}^{(1)}. \tag{2.14}$$

We can justify $\boldsymbol{P}^{(2)}\boldsymbol{D}^{(2)} \approx \boldsymbol{I}_{N+1}$ in a very similar fashion. □

Remark 2.1. To have a better understanding of the above approximate inverse, we derive a formula for the error remainder. More precisely, let $I_N^H : C(\mathbb{R}) \to \mathcal{P}_N(\mathbb{R})$ be the Lagrange interpolation at the Hermite–Gauss points $\{x_j\}_{j=0}^N$. Accordingly, we can define the interpolation associated with the Hermite functions: $\hat{I}_N^H u = e^{-x^2/2} I_N^H(u\, e^{x^2/2}) \in \widehat{\mathcal{P}}_N(\mathbb{R})$. Thus, we can understand (2.13) as the approximation of h_j' by its interpolant $\hat{I}_N^H h_j'$. Moreover, we can derive a computable error formula. Indeed, we obtain from (2.7) that

$$\begin{aligned} h_j'(x) - \sum_{k=0}^{N} h_j'(x_k)h_k(x) &= h_j'(x) - \hat{I}_N^H h_j'(x) \\ &= e^{(x_j^2-x^2)/2}(l_j'(x) - xl_j(x)) - e^{(x_j^2-x^2)/2} I_N^H(l_j'(x) - xl_j(x)) \\ &= e^{(x_j^2-x^2)/2}\big(I_N^H(xl_j(x)) - xl_j(x)\big) = (x_j - x)h_j(x), \end{aligned}$$

where in the last step, we used the property $I_N^H\phi = \phi$ for any $\phi \in \mathcal{P}_N(\mathbb{R})$, and $I_N^H(xl_j(x)) = \sum_{i=0}^N x_i l_j(x_i) l_i(x) = x_j l_j(x)$. Thus, by (2.13) and (2.14), we have

$$\mathcal{E}_j^H(x_i) =: \delta_{ij} - \sum_{k=0}^{N} p_k^{(1)}(x_i)\, d_{kj}^{(1)} = \int_{-\infty}^{x_i}(x_j - t)h_j(t)\,dt, \quad 0 \le i, j \le N. \tag{2.15}$$

That is, $\boldsymbol{I}_{N+1} - \boldsymbol{P}^{(1)}\boldsymbol{D}^{(1)} = \boldsymbol{\mathcal{E}}^H$ with the entries $\boldsymbol{\mathcal{E}}_{ij}^H = \mathcal{E}_j^H(x_i)$ for $0 \le i, j \le N$. However, it seems nontrivial to derive the explicit order of convergence. The numerical illustration in Fig. 2.3 (left) indicates the convergence rate is $\|\boldsymbol{\mathcal{E}}^H\|_\infty = \max_{i,j}|\boldsymbol{\mathcal{E}}_{ij}^H| = O(N^{-1})$ roughly.

A similar analysis can be conducted for the second-order differentiation matrix.

Consider the Hermite collocation method for $-u''(x) + u(x) = f(x)$ whose solution decays to zero at infinity. Then we know from (2.10) that the conditioning of the corresponding coefficient matrix: $-\boldsymbol{D}^{(2)} + \boldsymbol{I}_{N+1}$ behaves like $O(N)$. Using the approximate inverse as a preconditioner, we have the coefficient matrix of the linear system:

$$\boldsymbol{R} := \boldsymbol{P}^{(2)}\big(-\boldsymbol{D}^{(2)} + \boldsymbol{I}_{N+1}\big) \approx -\boldsymbol{I}_{N+1} + \boldsymbol{P}^{(2)}. \tag{2.16}$$

In view of (2.12), the eigenvalues of $\boldsymbol{R}$ behave like

$$\lambda_j(\boldsymbol{R}) \approx -1 + \lambda_j^{-1}(\boldsymbol{D}^{(2)}), \quad 0 \le j \le N. \tag{2.17}$$

Then by (2.10),

$$\min_j|\lambda_j(\boldsymbol{R})| = O(1), \quad \max_j|\lambda_j(\boldsymbol{R})| = O(N), \quad \mathrm{Cond}(\boldsymbol{R}) = O(N). \tag{2.18}$$

Observe that the preconditioning by the "approximate" inverse does not really relax the conditioning of the system, due to that the smallest eigenvalues decay to zero at a rate as in (2.9) and (2.10), as opposite to the Legendre and Chebyshev cases in [22].

2.2. Laguerre functions and Laguerre collocation differentiation matrices

Let $L_k(x)$, $x \in \mathbb{R}^+ := (0, \infty)$ be the Laguerre polynomial of degree k satisfying

$$\int_{\mathbb{R}^+} L_k(x)L_l(x)e^{-x}\mathrm{d}x = \delta_{kl}. \tag{2.19}$$

They are also the eigenfunctions of the Sturm–Liouville equation:

$$xL_k''(x) + (1-x)L_k'(x) + kL_k(x) = 0, \tag{2.20}$$

and note that $L_k(0) = 1$, and

$$L_k(x) = L_k'(x) - L_{k+1}'(x), \quad k \ge 0. \tag{2.21}$$

Define the corresponding Laguerre function as

$$\widehat{L}_k(x) = e^{-x/2}L_k(x), \quad k \ge 0. \tag{2.22}$$

Then by (2.21), we have

$$\frac{1}{2}\widehat{L}_{k+1}(x) + \frac{1}{2}\widehat{L}_k(x) = \widehat{L}_k'(x) - \widehat{L}_{k+1}'(x). \tag{2.23}$$

Let $\mathcal{P}_N(\mathbb{R}^+)$ be the set of all polynomials of degree at most N on $\mathbb{R}^+$, and

$$\widehat{\mathcal{P}}_N(\mathbb{R}^+) = \mathrm{span}\big\{\widehat{L}_0(x), \widehat{L}_1(x), \ldots, \widehat{L}_N(x)\big\} = \big\{u : u = e^{-x/2}v,\ v \in \mathcal{P}_N(\mathbb{R}^+)\big\}. \tag{2.24}$$

Recall that the Laguerre–Gauss–Radau (LGR) nodes: $\{x_j\}_{j=0}^N$ (arranged in ascending order) are zeros of $xL_{N+1}'(x)$ and by [6, (7.36)],

$$\int_{\mathbb{R}^+} p(x)q(x)\mathrm{d}x = \sum_{j=0}^{N} p(x_j)q(x_j)\hat{\omega}_j, \quad \hat{\omega}_j = \frac{1}{(N+1)\widehat{L}_N^2(x_j)}, \tag{2.25}$$

where $p \in \widehat{\mathcal{P}}_L(\mathbb{R}^+)$ and $q \in \widehat{\mathcal{P}}_M(\mathbb{R}^+)$ with $L + M \le 2N$. Let $\{\hat{l}_j\}_{j=0}^N$ be the usual Lagrange interpolating basis polynomials at LGR points $\{x_j\}_{j=0}^N$, and define the corresponding basis associated with Laguerre functions as

$$\hat{h}_j(x) = e^{(x_j - x)/2}\hat{l}_j(x) \in \widehat{\mathcal{P}}_N(\mathbb{R}^+), \quad \hat{h}_j(x_i) = \delta_{ij}, \quad 0 \le i, j \le N. \tag{2.26}$$

Introduce the collocation differentiation matrices:

$$\widehat{\boldsymbol{D}}^{(m)} = \big(\hat{d}_{ij}^{(m)} := \hat{h}_j^{(m)}(x_i)\big)_{0\le i,j\le N}, \quad \widehat{\boldsymbol{D}}_{\mathrm{in}}^{(m)} = \big(\hat{d}_{ij}^{(m)}\big)_{1\le i,j\le N}.$$

Like (2.9) and (2.10), we have the following behaviours (cf. [42]):

$$\min_j|\lambda_j| = O\big(N^{-1}\big), \quad \max_j|\lambda_j| = O(N), \quad \mathrm{Cond}(\widehat{\boldsymbol{D}}_{\mathrm{in}}^{(1)}) = O(N^2), \tag{2.27}$$

and

$$\min_j|\lambda_j| = O\big(N^{-2}\big), \quad \max_j|\lambda_j| = O(N^2), \quad \mathrm{Cond}(\widehat{\boldsymbol{D}}_{\mathrm{in}}^{(2)}) = O(N^4). \tag{2.28}$$

The numerical illustrations in Fig. 2.2 agree with the above estimates.

As with the Hermite case, we can find the approximate inverse of the Laguerre collocation differentiation matrices through integration. To do this, we introduce the Lagrange interpolating basis at the "interior" LGR points $\{x_j\}_{j=1}^N$:

$$\tilde{l}_j(x) = \frac{x_j}{x}\hat{l}_j(x), \quad \tilde{h}_j(x) = e^{(x_j-x)/2}\tilde{l}_j(x) \in \widehat{\mathcal{P}}_{N-1}(\mathbb{R}^+), \quad 1 \le i, j \le N. \tag{2.29}$$

Like (2.11), we introduce

$$g_j^{(1)}(x) = \int_0^x \tilde{h}_j(t)\,\mathrm{d}t, \quad 1 \le j \le N, \tag{2.30}$$

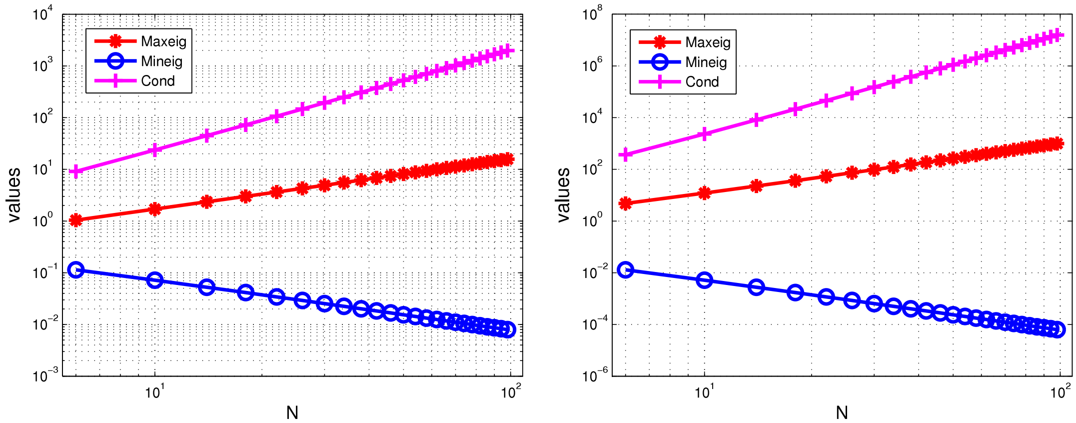

Fig. 2.2. The modulus of the largest, smallest eigenvalues and condition numbers in log–log scale. Left: $\widehat{\boldsymbol{D}}_{\text{in}}^{(1)}$; Right: $\widehat{\boldsymbol{D}}_{\text{in}}^{(2)}$.

and

$$g_j^{(2)}(x) = \frac{1}{2}\int_0^x (x-t)\tilde{h}_j(t)\,\mathrm{d}t + \frac{1}{2}\int_x^\infty (t-x)\tilde{h}_j(t)\,\mathrm{d}t - \frac{1}{2}\int_0^\infty (x+t)\tilde{h}_j(t)\,\mathrm{d}t, \tag{2.31}$$

for $1 \le j \le N$. They can be computed efficiently by using Lemma 3.1 and the three-term recurrence formula of the Laguerre functions.

We have the following approximate inverse. Here, we omit the proof as it is very similar to that of Proposition 2.1.

Proposition 2.2. *Let* $\{g_j^{(1)}, g_j^{(2)}\}$ *be defined as in* (2.30) *and* (2.31)*, and define the matrices* $\boldsymbol{G}^{(1)}, \boldsymbol{G}^{(2)}$ *with the ijth entries:* $g_j^{(1)}(x_i), g_j^{(2)}(x_i)$*, respectively. Then we have*

$$\boldsymbol{G}^{(1)}\widehat{\boldsymbol{D}}_{\text{in}}^{(1)} \approx \boldsymbol{I}_N, \quad \boldsymbol{G}^{(2)}\widehat{\boldsymbol{D}}_{\text{in}}^{(2)} \approx \boldsymbol{I}_N. \tag{2.32}$$

Remark 2.2. Like Remark 2.1, we can understand the above approximate inverse from the perspectives of interpolation approximation and the error formula. It is clear that by (2.26) and (2.29),

$$\hat{h}_j'(x) = e^{(x_j-x)/2}\Big(\hat{l}_j'(x) - \frac{1}{2}\hat{l}_j(x)\Big), \quad \hat{h}_j'(x_k) = e^{(x_j-x_k)/2}\Big(\hat{l}_j'(x_k) - \frac{1}{2}\delta_{kj}\Big).$$

Thus, we can write and derive that

$$\begin{aligned}\hat{h}_j'(x) - \sum_{k=1}^N \hat{h}_j'(x_k)\tilde{h}_k(x) &= \hat{h}_j'(x) - \frac{e^{(x_j-x)/2}}{x}\sum_{k=1}^N x_k\hat{l}_j'(x_k)\hat{l}_k(x) + \frac{1}{2}\tilde{h}_j(x)\\ &= \hat{h}_j'(x) - \frac{e^{(x_j-x)/2}}{x}x\hat{l}_j'(x) + \frac{1}{2}\tilde{h}_j(x) = \frac{1}{2}\big(\tilde{h}_j(x) - \hat{h}_j(x)\big),\end{aligned}$$

where we used the fact $x_0 = 0$, and the Laguerre–Gauss–Radau interpolation is exact for any polynomial in $\widehat{\mathcal{P}}_N(\mathbb{R}^+)$. This implies $\boldsymbol{I}_N - \boldsymbol{G}^{(1)}\widehat{\boldsymbol{D}}_{\text{in}}^{(1)} = \boldsymbol{\mathcal{E}}^L$ with the entries given by

$$\mathcal{E}_{ij}^L := \frac{1}{2}\int_0^{x_i}\big(\tilde{h}_j(t) - \hat{h}_j(t)\big)\mathrm{d}t = \frac{1}{2}\int_0^{x_i}\Big(\frac{x_j}{t} - 1\Big)\hat{h}_j(t)\,\mathrm{d}t, \quad 1 \le i, j \le N.$$

Like the Hermite case, we observe from Fig. 2.3 (right) that $\|\boldsymbol{\mathcal{E}}^L\|_\infty = \max_{i,j}|\mathcal{E}_{ij}^L| = O(N^{-1})$ approximately.

Similarly, we can analyse the second approximate inverse in (2.32).

Consider $-u''(x) + u(x) = f(x)$ with $u(0) = 0$ and $u(x) \to 0$ as $x \to \infty$. From (2.28), we know the condition numbers of the coefficient matrix: $\boldsymbol{H} = -\widehat{\boldsymbol{D}}_{\text{in}}^{(2)} + \boldsymbol{I}_N$ of the usual collocation method growing like $O(N^2)$. We can precondition the matrix by using the approximate inverse:

$$\boldsymbol{E} := \boldsymbol{G}^{(2)}\big(-\widehat{\boldsymbol{D}}_{\text{in}}^{(2)} + \boldsymbol{I}_N\big) \approx -\boldsymbol{I}_N + \boldsymbol{G}^{(2)}. \tag{2.33}$$

According to (2.32), the eigenvalues are

$$\lambda_j(\boldsymbol{E}) \approx -1 + \lambda_j^{-1}(\widehat{\boldsymbol{D}}_{\text{in}}^{(2)}), \quad 1 \le j \le N, \tag{2.34}$$

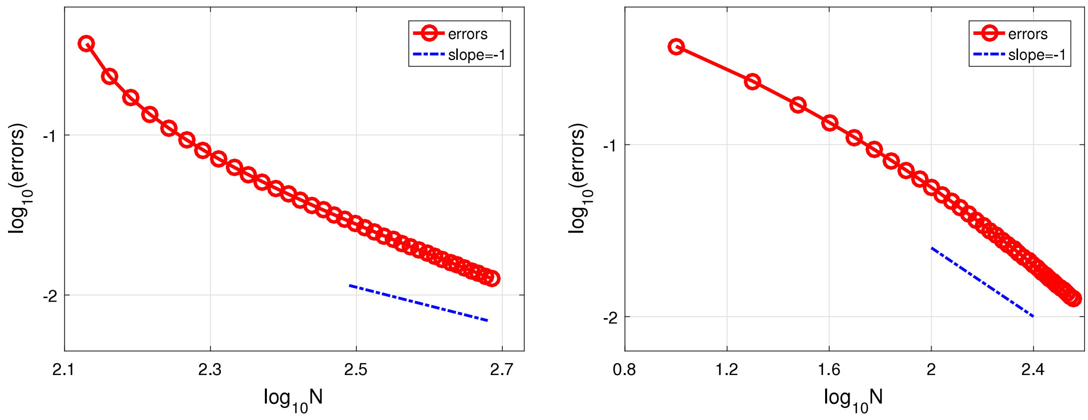

Fig. 2.3. The convergence rate of $\|\boldsymbol{\varepsilon}^H\|_\infty$ in Remark 2.1 and $\|\boldsymbol{\varepsilon}^L\|_\infty$ in Remark 2.2 in log–log scale. Left: Hermite case. Right: Laguerre case.

so we have

$$\min_j|\lambda_j(\boldsymbol{E})| = O(1), \quad \max_j|\lambda_j(\boldsymbol{E})| = O(N^2), \quad \mathrm{Cond}(\boldsymbol{E}) = O(N^2). \tag{2.35}$$

Similar to the Hermite case, the smallest eigenvalues in (2.27) and (2.28) decay with respect to N, so the above preconditioning does not relax the conditioning of the original collocation system, which should be in contrast with the Chebyshev and Legendre cases in the finite domain (cf. [22]).

3. New basis functions and their properties

Motivated by previous studies, we find it is necessary to use the inverse of $-\boldsymbol{D}^{(2)} + \nu \boldsymbol{I}_{N+1}$ in (2.16) and $-\widehat{\boldsymbol{D}}^{(2)}_{\mathrm{in}} + \lambda \boldsymbol{I}_N$ in (2.33) as preconditioners, which can lead to well-conditioned collocation schemes for general second-order equations. In what follows, we explicitly compute their approximate inverse in an efficient and stable manner, and demonstrate the advantages of this new approach.

3.1. New basis functions on the whole line

Denote the following second-order differential operator by

$$\mathcal{L}_\nu[u](x) = u''(x) - \nu^2 u(x), \quad x \in \mathbb{R}, \quad \nu > 0. \tag{3.1}$$

Our goal is to explicitly construct a basis $\{Q_j\}_{j=0}^N$ such that

$$\mathcal{L}_\nu[Q_j](x) = h_j(x), \quad 0 \le j \le N; \quad Q_j(x) \to 0 \;\text{ as }\; |x| \to \infty, \tag{3.2}$$

which implies

$$\mathcal{L}_\nu[Q_j](x_i) = \delta_{ij}, \quad 0 \le i, j \le N. \tag{3.3}$$

Define the matrices

$$\boldsymbol{Q}^{(k)} = \big(q_{ij}^{(k)}\big)_{0\le i,j\le N}, \quad \text{where} \;\; q_{ij}^{(k)} = Q_j^{(k)}(x_i). \tag{3.4}$$

Then there holds

$$\boldsymbol{Q}^{(2)} - \nu^2 \boldsymbol{Q} = \boldsymbol{I}_{N+1}, \quad \boldsymbol{Q} = \boldsymbol{Q}^{(0)}. \tag{3.5}$$

In other words, the collocation matrix associated with $\mathcal{L}_\nu[u](x)$ becomes identity matrix.

Below, we present the explicit formulas for computing the new basis $\{Q_j\}_{j=0}^N$.

Theorem 3.1. *Let $\{x_j, \omega_j\}_{j=0}^N$ be the Hermite–Gauss quadrature nodes and weights. Then*

$$Q_j(x) = -\frac{1}{2\nu}\sum_{k=0}^N \omega_j \widehat{H}_k(x_j)\left\{\mathcal{I}_\nu^-[\widehat{H}_k](x) + \mathcal{I}_\nu^+[\widehat{H}_k](x)\right\}, \quad 0 \le j \le N, \tag{3.6}$$

where

$$\mathcal{I}_\nu^-[\widehat{H}_k](x) = \int_{-\infty}^{x} e^{-\nu(x-y)}\widehat{H}_k(y)\,\mathrm{d}y, \quad \mathcal{I}_\nu^+[\widehat{H}_k](x) = \int_{x}^{\infty} e^{-\nu(y-x)}\widehat{H}_k(y)\,\mathrm{d}y, \tag{3.7}$$

satisfying

$$\mathcal{I}_\nu^+[\widehat{H}_k](x) = (-1)^k \mathcal{I}_\nu^-[\widehat{H}_k](-x). \tag{3.8}$$

Moreover, we have the following recurrence relation:

$$\begin{aligned}
&\sqrt{\frac{k+1}{2}}\,\mathcal{I}_\nu^-[\widehat{H}_{k+1}](x) = \nu\mathcal{I}_\nu^-[\widehat{H}_k](x) + \sqrt{\frac{k}{2}}\mathcal{I}_\nu^-[\widehat{H}_{k-1}](x) - \widehat{H}_k(x), \quad k \ge 1,\\
&\mathcal{I}_\nu^-[\widehat{H}_0](x) = \frac{\pi^{\frac14}}{\sqrt{2}} e^{\frac12\nu^2-\nu x}\Big(1+\mathrm{erf}\Big(\frac{x-\nu}{\sqrt2}\Big)\Big),\\
&\mathcal{I}_\nu^-[\widehat{H}_1](x) = -\sqrt{2}\pi^{-\frac14} e^{-\frac{x^2}{2}} + \pi^{\frac14}\nu e^{\frac12\nu^2-\nu x}\Big(1+\mathrm{erf}\Big(\frac{x-\nu}{\sqrt2}\Big)\Big).
\end{aligned} \tag{3.9}$$

Proof. Let $\{h_j\}$ be the interpolating basis defined in (2.7). Solving (3.2) leads to

$$\begin{aligned}
Q_j(x) &= C_1 e^{-\nu x} + C_2 e^{\nu x} - \frac{e^{-\nu x}}{2\nu}\int_{-\infty}^{x} e^{\nu y} h_j(y)\mathrm{d}y + \frac{e^{\nu x}}{2\nu}\int_{-\infty}^{x} e^{-\nu y}h_j(y)\mathrm{d}y\\
&= e^{-\nu x}\Big(C_1 - \frac{1}{2\nu}\int_{-\infty}^{x} e^{\nu y}h_j(y)\,\mathrm{d}y\Big) + e^{\nu x}\Big(C_2 + \frac{1}{2\nu}\int_{-\infty}^{x} e^{-\nu y}h_j(y)\,\mathrm{d}y\Big).
\end{aligned} \tag{3.10}$$

As $Q_j(x) \to 0$ at infinity, we infer that

$$C_1 = 0, \quad C_2 = -\frac{1}{2\nu}\int_{-\infty}^{\infty} e^{-\nu y}h_j(y)\mathrm{d}y.$$

Substituting C_1 and C_2 into (3.10), we find

$$Q_j(x) = -\frac{1}{2\nu}\left(\mathcal{I}_\nu^-[h_j](x) + \mathcal{I}_\nu^+[h_j](x)\right), \quad 0 \le j \le N, \tag{3.11}$$

which, together with (2.8), leads to (3.6).

By (2.2), we have

$$\begin{aligned}
\mathcal{I}_\nu^-[\widehat{H}_k](-x) &= \int_{-\infty}^{-x} e^{-\nu(-x-y)}\widehat{H}_k(y)\mathrm{d}y = \int_{x}^{\infty} e^{-\nu(y-x)}(-1)^k\widehat{H}_k(y)\mathrm{d}y\\
&= (-1)^k\int_{x}^{\infty} e^{-\nu(y-x)}\widehat{H}_k(y)\mathrm{d}y = (-1)^k\,\mathcal{I}_\nu^+[\widehat{H}_k](x),
\end{aligned} \tag{3.12}$$

which yields (3.8).

Finally, we show (3.9). Using (2.4), (3.7) and integration by parts, we obtain

$$\sqrt{\frac{k}{2}}\mathcal{I}_\nu^-[\widehat{H}_{k-1}](x) - \sqrt{\frac{k+1}{2}}\mathcal{I}_\nu^-[\widehat{H}_{k+1}](x) = \int_{-\infty}^{x} e^{-\nu(x-y)}\widehat{H}_k'(y)\mathrm{d}y = \widehat{H}_k(x) - \nu\mathcal{I}_\nu^-[\widehat{H}_k](x).$$

Next, by the definition (3.7) and a direct calculation, we obtain

$$\begin{aligned}
\mathcal{I}_\nu^-[\widehat{H}_0](x) &= \int_{-\infty}^{x} e^{-\nu(x-y)}\widehat{H}_0(y)dy = \pi^{-\frac14}\int_{-\infty}^{x} e^{-\nu(x-y)}e^{-\frac{y^2}{2}}\,dy\\
&= \pi^{-\frac14}e^{\frac12\nu^2-\nu x}\int_{-\infty}^{x} e^{-\frac12(y-\nu)^2}dy = \pi^{-\frac14}e^{\frac12\nu^2-\nu x}\int_{-\infty}^{x-\nu} e^{-\frac12 y^2}dy\\
&= \pi^{-\frac14}e^{\frac12\nu^2-\nu x}\Big(\frac{\sqrt{2\pi}}{2} + \int_0^{x-\nu} e^{-\frac12 y^2}dy\Big)\\
&= \pi^{-\frac14}e^{\frac12\nu^2-\nu x}\Big(\frac{\sqrt{2\pi}}{2} + \sqrt2\int_0^{\frac{x-\nu}{\sqrt2}} e^{-y^2}dy\Big)\\
&= \frac{\pi^{\frac14}}{\sqrt2}e^{\frac12\nu^2-\nu x}\Big(1+\mathrm{erf}\Big(\frac{x-\nu}{\sqrt2}\Big)\Big),
\end{aligned}$$

and

$$\begin{aligned}\mathcal{I}_\nu^-[\widehat{H}_1](x) &= \int_{-\infty}^x e^{-\nu(x-y)}\widehat{H}_1(y)dy = \sqrt{2}\pi^{-\frac14}\int_{-\infty}^x e^{-\nu(x-y)}ye^{-\frac{y^2}{2}}dy\\ &= -\sqrt{2}\pi^{-\frac14}e^{-\nu(x-y)}e^{-\frac{y^2}{2}}\Big|_{-\infty}^x + \sqrt{2}\pi^{-\frac14}\nu\int_{-\infty}^x e^{-\nu(x-y)}e^{-\frac{y^2}{2}}dy\\ &= -\sqrt{2}\pi^{-\frac14}e^{-\frac{x^2}{2}} + \sqrt{2}\nu\mathcal{I}_\nu^-[\widehat{H}_0](x)\\ &= -\sqrt{2}\pi^{-\frac14}e^{-\frac{x^2}{2}} + \pi^{\frac14}\nu e^{\frac12\nu^2-\nu x}\Big(1+\mathrm{erf}\Big(\frac{x-\nu}{\sqrt{2}}\Big)\Big).\end{aligned}$$

This ends the proof. □

3.2. New basis functions on the half line

Consider the second-order linear differential operator on $\mathbb{R}^+$:

$$\mathscr{F}_\lambda[u](x) = u''(x) - \lambda^2 u(x), \quad x \in \mathbb{R}^+, \tag{3.13}$$

where the constant $\lambda > 0$. The main objective is to construct a new basis $\{S_j\}_{j=0}^N$ such that

- for $1 \le j \le N$,

$$\mathscr{F}_\lambda[S_j](x) = \tilde{h}_j(x), \quad x \in \mathbb{R}^+; \quad S_j(0) = 0; \tag{3.14}$$

- for $j = 0$,

$$\mathscr{F}_\lambda[S_0](x) = 0, \quad x \in \mathbb{R}^+; \quad S_0(0) = 1, \tag{3.15}$$

where $\{\tilde{h}_j\}$ are the interpolating basis defined in (2.29). With this, taking $x = x_i$ in (3.14) and (3.15) yields that

$$\begin{cases}\mathscr{F}_\lambda[S_j](x_i) = \delta_{ij}, \quad 1 \le i, j \le N; \quad S_j(0) = 0, \quad 1 \le j \le N;\\ \mathscr{F}_\lambda[S_0](x_i) = 0, \quad 1 \le i \le N, \quad S_0(0) = 1.\end{cases} \tag{3.16}$$

Define

$$\boldsymbol{S}^{(k)} = \big(s_{ij}^{(k)} = S_j^{(k)}(x_i)\big)_{1\le i,j\le N}, \quad \boldsymbol{S} = \boldsymbol{S}^{(0)}. \tag{3.17}$$

Then there holds

$$\boldsymbol{S}^{(2)} - \lambda^2\boldsymbol{S} = \boldsymbol{I}_N. \tag{3.18}$$

We next propose an efficient algorithm for computing the new basis, and first derive the following important formula.

Lemma 3.1. *Let $\{x_j, \hat{\omega}_j\}_{j=0}^N$ be the LGR points and quadrature weights as in (2.25). Then $\{\tilde{h}_j\}_{j=1}^N$ has the representation:*

$$\tilde{h}_j(x) = \sum_{k=0}^{N-1} \nu_k^j \widehat{L}_k(x), \quad 1 \le j \le N; \quad \nu_k^j = -\frac{\hat{\omega}_0}{\widehat{L}_{N+1}(x_j)} + \hat{\omega}_j\widehat{L}_k(x_j). \tag{3.19}$$

Proof. By the orthogonality (2.19) and (2.22),

$$\nu_k^j = \int_{\mathbb{R}^+} \tilde{h}_j(x)\widehat{L}_k(x)\,\mathrm{d}x = \tilde{h}_j(0)\widehat{L}_k(0)\hat{\omega}_0 + \widehat{L}_k(x_j)\hat{\omega}_j, \tag{3.20}$$

where we used the property: $\tilde{h}_j(x_i) = \delta_{ij}$ for $1 \le i, j \le N$. Thus, it remains to calculate $\tilde{h}_j(0)$. As the interior LGR points $\{x_j\}_{j=1}^N$ are zeros of $L'_{N+1}(x)$, we have

$$\tilde{l}_j(0) = \frac{L'_{N+1}(x)}{(x-x_j)\,L''_{N+1}(x_j)}\bigg|_{x=0}. \tag{3.21}$$

By (2.20),

$$L'_{N+1}(0) = -(N+1), \quad x_j L''_{N+1}(x_j) = -(N+1)L_{N+1}(x_j), \quad 1 \le j \le N. \tag{3.22}$$

Then $\tilde{h}_j(0) = -(\widehat{L}_{N+1}(x_j))^{-1}$. Thus, the desired formula (3.19) follows from the above. □

Like Theorem 3.1, we have the following algorithm for computing the basis efficiently.

Theorem 3.2. *We have* $S_0(x) = e^{-\lambda x}$, *and*

$$S_j(x) = -\frac{1}{2\lambda}\sum_{k=0}^{N-1} \nu_k^j \left\{ I_\lambda^-[\widehat{L}_k](x) + I_\lambda^+[\widehat{L}_k](x) - I_\lambda^\infty[\widehat{L}_k](x)\right\}, \quad 1 \le j \le N, \tag{3.23}$$

where $\{\nu_k^j\}$ *are given in* Lemma 3.1, *and*

$$\begin{aligned} &I_\lambda^-[\widehat{L}_k](x) = \int_0^x e^{-\lambda(x-y)}\widehat{L}_k(y)\,\mathrm{d}y, \quad I_\lambda^+[\widehat{L}_k](x) = \int_x^\infty e^{-\lambda(y-x)}\widehat{L}_k(y)\,\mathrm{d}y, \\ &I_\lambda^\infty[\widehat{L}_k](x) = \int_0^\infty e^{-\lambda(x+y)}\widehat{L}_k(y)\,\mathrm{d}y. \end{aligned} \tag{3.24}$$

We have the recurrence formulas:

$$I_\lambda^-[\widehat{L}_k](x) = \frac{2\lambda-1}{2\lambda+1}\, I_\lambda^-[\widehat{L}_{k+1}](x) + \frac{2}{2\lambda+1}(\widehat{L}_k(x) - \widehat{L}_{k+1}(x)), \tag{3.25}$$

$$I_\lambda^+[\widehat{L}_{k+1}](x) = \frac{2\lambda-1}{2\lambda+1}\, I_\lambda^+[\widehat{L}_k](x) + \frac{2}{2\lambda+1}(\widehat{L}_{k+1}(x) - \widehat{L}_k(x)), \tag{3.26}$$

with $I_\lambda^+[\widehat{L}_0](x) = 2e^{-x/2}/(2\lambda+1)$. *Moreover, we have the exact formula:*

$$I_\lambda^\infty[\widehat{L}_k](x) = \frac{2(2\lambda-1)^k}{(2\lambda+1)^{k+1}} e^{-\lambda x}. \tag{3.27}$$

Proof. It is evident that $S_0(x) = e^{-\lambda x}$ is the unique solution to (3.15). Solving (3.14) directly, we find that

$$S_j(x) = \frac{1}{2\lambda} I_\lambda^\infty[\tilde{h}_j](x) - \frac{1}{2\lambda} I_\lambda^-[\tilde{h}_j](x) - \frac{1}{2\lambda} I_\lambda^+[\tilde{h}_j](x), \quad 1 \le j \le N. \tag{3.28}$$

Substituting the formula of $\tilde{h}_j$ in Lemma 3.1 into the above leads to (3.23).

By (2.23) and (3.24), we derive from a direct calculation that

$$\begin{aligned} \frac{1}{2}\left\{ I_\lambda^+[\widehat{L}_k](x) + I_\lambda^+[\widehat{L}_{k+1}](x)\right\} &= \int_x^\infty e^{-\lambda(y-x)}\left\{\widehat{L}_k'(y) - \widehat{L}_{k+1}'(y)\right\}\mathrm{d}y \\ &= e^{-\lambda(y-x)}\left\{\widehat{L}_k(y) - \widehat{L}_{k+1}(y)\right\}\Big|_x^\infty + \lambda I_\lambda^+[\widehat{L}_k](x) - \lambda I_\lambda^+[\widehat{L}_{k+1}](x) \\ &= \lambda\, I_\lambda^+[\widehat{L}_k](x) - \lambda\, I_\lambda^+[\widehat{L}_{k+1}](x) + \widehat{L}_{k+1}(x) - \widehat{L}_k(x), \end{aligned} \tag{3.29}$$

which implies (3.26). It is clear that

$$I_\lambda^+[\widehat{L}_0](x) = \int_x^\infty e^{-\lambda(y-x)} e^{-y/2} dy = \frac{2}{2\lambda+1} e^{-x/2}.$$

The formula (3.25) can be derived in a very similar fashion.

Following the same lines in (3.29), we can show that

$$I_\lambda^\infty[\widehat{L}_{k+1}](x) = \frac{2\lambda-1}{2\lambda+1}\, I_\lambda^\infty[\widehat{L}_k](x) = \cdots = \left(\frac{2\lambda-1}{2\lambda+1}\right)^{k+1} I_\lambda^\infty[\widehat{L}_0](x) = \frac{2(2\lambda-1)^{k+1}}{(2\lambda+1)^{k+2}} e^{-\lambda x}. \tag{3.30}$$

This ends the proof. □

Interestingly, when $\lambda = 1/2$, the new basis takes a much simpler form, which follows from Theorem 3.2 immediately.

Corollary 3.1. *For* $\lambda = 1/2$, *we have*

$$S_j(x) = \sum_{k=0}^{N-1} \nu_k^j \left\{ \widehat{L}_{k+1}(x) - 2\widehat{L}_k(x) + \widehat{L}_{k-1}(x)\right\}, \quad 1 \le j \le N, \tag{3.31}$$

where $\widehat{L}_{-1}(x) = 0$.

Remark 3.1. Observe from (3.25) that it is necessary to implement the recurrence formula backwards for slightly large λ. That is

$$I_\lambda^-[\widehat{L}_k](x) = \frac{2\lambda-1}{2\lambda+1}\, I_\lambda^-[\widehat{L}_{k+1}](x) + \frac{2}{2\lambda+1}(\widehat{L}_k(x) - \widehat{L}_{k+1}(x)), \quad k = N-1, \ldots, 0, \tag{3.32}$$

with the input $I_\lambda^-[\widehat{L}_N](x)$. In fact, the initial values at the LGR points $\{x_i\}_{i=1}^N$ can be calculated efficiently by the rapid deconvolution formula (see, e.g., [46]):

$$I_\lambda^-[\widehat{L}_N](x_i) = e^{-\lambda \Delta x_i} I_\lambda^-[\widehat{L}_N](x_{i-1}) + \int_{x_{i-1}}^{x_i} e^{-\lambda(x_i-y)} \widehat{L}_N(y)\,dy, \tag{3.33}$$

and $I_\lambda^-[\widehat{L}_N](x_0) = 0$, where $\Delta x_i = x_i - x_{i-1}$ for $1 \le i \le N$. As a result, we can use the Legendre–Gauss quadrature to compute the integral on $[x_{i-1}, x_i]$ accurately.

3.3. Important properties

The matrix $\boldsymbol{Q}$ in (3.4) generated from the new basis in Theorem 3.1 is an approximate inverse of the matrix of the Hermite collocation method $\mathcal{L}_\nu[u](x) = f(x), x \in \mathbb{R}$ with $u(x) \to 0$ as $|x| \to \infty$. The Hermite–Gauss collocation scheme is to find $u_N \in \widehat{\mathcal{P}}_N(\mathbb{R})$ such that

$$\mathcal{L}_\nu[u_N](x_j) = f(x_j), \quad 0 \le j \le N. \tag{3.34}$$

Under the Lagrange interpolating basis functions $\{h_j\}$ in (2.7), the matrix form of (3.34) is

$$\boldsymbol{L}\,\boldsymbol{u} = \big(\boldsymbol{D}^{(2)} - \nu^2 \boldsymbol{I}_{N+1}\big)\boldsymbol{u} = \boldsymbol{f}, \tag{3.35}$$

where

$$\boldsymbol{u} = \big(u_N(x_0), u_N(x_1), \ldots, u_N(x_N)\big)^t, \quad \boldsymbol{f} = \big(f(x_0), f(x_1), \ldots, f(x_N)\big)^t. \tag{3.36}$$

Proposition 3.1. *Let $\boldsymbol{L} = \boldsymbol{D}^{(2)} - \nu^2 \boldsymbol{I}_{N+1}$ and $\boldsymbol{Q}$ be the matrix defined in (3.4). Then we have $\boldsymbol{QL} \approx \boldsymbol{I}_{N+1} \approx \boldsymbol{LQ}$.*

Proof. Note that $\boldsymbol{Q}_j(x)$ can be well approximated by the interpolation:

$$Q_j(x) \approx \sum_{k=0}^N Q_j(x_k) h_k(x), \quad \text{so} \quad \mathcal{L}_\nu[Q_j](x) \approx \sum_{k=0}^N Q_j(x_k) \mathcal{L}_\nu[h_k](x).$$

Then by (3.3),

$$\delta_{ij} = \mathcal{L}_\nu[Q_j](x_k) \approx \sum_{k=0}^N Q_j(x_k) \mathcal{L}_\nu[h_k](x_i), \quad \text{so} \quad \boldsymbol{I}_{N+1} \approx \big(\boldsymbol{D}^{(2)} - \nu^2 \boldsymbol{I}_{N+1}\big)\boldsymbol{Q}.$$

Thus, $\boldsymbol{LQ} \approx \boldsymbol{I}_{N+1}$. Similarly, consider the approximation:

$$\mathcal{L}_\nu[h_j](x) \approx \sum_{k=0}^N \mathcal{L}_\nu[h_j](x_k) h_k(x), \quad \text{so} \quad h_j(x) \approx \sum_{k=0}^N \mathcal{L}_\nu[h_j](x_k) \mathcal{L}_\nu^{-1}[h_k](x).$$

Hence, by (3.2) and taking $x = x_i$, we claim that $\boldsymbol{QL} \approx \boldsymbol{I}_{N+1}$. $\square$

The above important property is also valid for the Laguerre case. Similarly, we consider the Laguerre collocation method for $\mathscr{F}_\lambda[u](x) = f(x), x \in \mathbb{R}^+$ with $u(0) = 0$ and $u(x) \to 0$ as $x \to \infty$. Then the collocation matrix is $\boldsymbol{F} = \widehat{\boldsymbol{D}}_{\rm in}^{(2)} - \lambda^2 \boldsymbol{I}_N$ as in (2.33).

Proposition 3.2. *Let $\boldsymbol{F} = \widehat{\boldsymbol{D}}_{\rm in}^{(2)} - \lambda^2 \boldsymbol{I}_N$ and $\boldsymbol{S}$ be the matrix defined in (3.17). Then we have $\boldsymbol{SF} \approx \boldsymbol{I}_N \approx \boldsymbol{FS}$.*

Let $\{\lambda_j\}_{j=0}^N$ be the eigenvalues of $\boldsymbol{QL}$. We plot in Fig. 3.1 the errors: $\max_j|\lambda_j - 1|$ and $\min_j|\lambda_j - 1|$ against N in log-scale for both Hermite and Laguerre cases. We observe that all their eigenvalues are concentrated around one for slightly large N.

As a very important special case, when $\lambda = 1/2$, the new basis in Corollary 3.1 offers the exact inverse.

Proposition 3.3. *For $\lambda = 1/2$, let $\boldsymbol{F}_* = \widehat{\boldsymbol{D}}_{\rm in}^{(2)} - \frac{1}{4}\boldsymbol{I}_N$, and we have*

$$\boldsymbol{SF}_* = \boldsymbol{F}_*\boldsymbol{S} = \boldsymbol{I}_N. \tag{3.37}$$

Proof. From Corollary 3.1, we know from (2.24) that $S_j \in \widehat{\mathcal{P}}_N(\mathbb{R}^+)$. Thus, we have

$$S_j(x) = \sum_{k=0}^N S_j(x_k)\hat{h}_k(x) = \sum_{k=1}^N S_j(x_k)\hat{h}_k(x), \quad 1 \le j \le N,$$

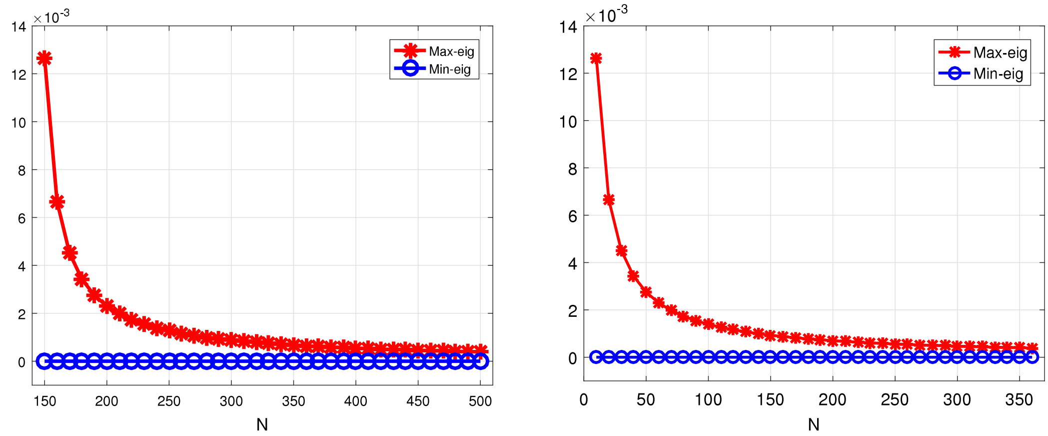

Fig. 3.1. The errors of $\max_j|\lambda_j - 1|$ and $\min_j|\lambda_j - 1|$ against N (note: $\{\lambda_j\}_{j=0}^N$ are the eigenvalues). Left: ***QL*** for Hermite case. Right: ***SF*** for Laguerre case.

where we used the fact: $S_j(x_0) = 0$. Thus, by (3.16),

$$\delta_{ij} = \mathscr{F}_{\frac{1}{2}}[S_j](x_i) = \sum_{k=1}^{N} S_j(x_k)\mathscr{F}_{\frac{1}{2}}[\hat{h}_k](x_i), \quad 1 \le j \le N.$$

This ends the proof. □

Remark 3.2. It is seen from Corollary 3.1 that the new basis $\{S_j\}$ with $\lambda = 1/2$ takes the simplest form and belong to $\widehat{\mathcal{P}}_N(\mathbb{R}^+)$. In fact, we can use it to precondition the matrix $\boldsymbol{F} = \widehat{\boldsymbol{D}}_{\rm in}^{(2)} - \lambda^2 \boldsymbol{I}_N$ with $\lambda \ne 1/2$. More precisely, we find from (3.37) that

$$\boldsymbol{SF} = \boldsymbol{S}\big\{\boldsymbol{F}_* + (1/4 - \lambda^2)\boldsymbol{I}_N\big\} = \boldsymbol{I}_N + (1/4 - \lambda^2)\boldsymbol{S}, \tag{3.38}$$

and the eigenvalues:

$$\lambda_j(\boldsymbol{S}) = \lambda_j(\boldsymbol{F}_*^{-1}) = \big(\lambda_j(\widehat{\boldsymbol{D}}_{\rm in}^{(2)}) - 1/4\big)^{-1}.$$

Thus, we infer from (2.28) that

$$\min_j|\lambda_j(\boldsymbol{S})| = O(N^{-2}), \quad \max_j|\lambda_j(\boldsymbol{S})| = O(1).$$

We find from (3.38) readily that $\lambda_j(\boldsymbol{SF}) = O(1)$ for all $1 \le j \le N$, so $\mathrm{Cond}(\boldsymbol{SF}) = O(1)$.

4. Applications and numerical results

In this section, we propose new collocation methods using the new basis for various PDEs in unbounded domains, and demonstrate the high accuracy and efficiency of the proposed approaches. More precisely, we consider BVPs in one and two dimensions, and time-dependent equations. Moreover, we develop a Legendre–Laguerre multi-domain collocation schemes using the integral basis in [22] and new basis herein to enhance the accuracy and resolution of the solver on the half line.

4.1. Illustrative examples

To demonstrate the idea, we consider the Hermite collocation schemes for the model problem on the whole line:

$$-u''(x) + r(x)u'(x) + s(x)u(x) = f(x), \quad x \in \mathbb{R}; \quad \lim_{|x|\to\infty} u(x) = 0, \tag{4.1}$$

where the given functions $r, s, f \in C(\mathbb{R})$. Let $\{x_i\}_{i=0}^N$ be the Hermite–Gauss points as before. Then the collocation scheme for (4.1) is to find $u_N \in \widehat{\mathcal{P}}_N(\mathbb{R})$ such that

$$-u_N''(x_i) + r(x_i)u_N'(x_i) + s(x_i)u_N(x_i) = f(x_i), \quad 0 \le i \le N. \tag{4.2}$$

Let $\{h_j\}_{j=0}^N$ be the Lagrange basis functions defined in (2.7). We expand the numerical solution of (4.1) as

$$u_N(x) = \sum_{j=0}^{N} u_N(x_j)h_j(x), \tag{4.3}$$

Table 4.1
Condition numbers of two schemes with $\beta = 2$ and $\nu = \frac{1}{2}$.

	$N = 20$	$N = 60$	$N = 100$	$N = 140$	$N = 180$
LCOL (4.4)	1.50E+02	4.61E+02	7.75E+02	1.09E+03	1.41E+03
BCOL (4.5)	6.1	21.9	40.6	60.8	82.1

and substitute it into (4.2), leading to

$$-\sum_{j=0}^{N} u_N(x_j)h_j''(x_i) + r(x_i)\sum_{j=0}^{N} u_N(x_j)h_j'(x_i) + s(x_i)\sum_{j=0}^{N} u_N(x_j)h_j(x_i) = f(x_i), \quad 0 \le i \le N.$$

Thus, the above equations can be written in the form of matrix as follows:

$$\left(-\boldsymbol{D}^{(2)} + \boldsymbol{\Sigma}_r \boldsymbol{D}^{(1)} + \boldsymbol{\Sigma}_s\right)\boldsymbol{u} = \boldsymbol{f}, \tag{4.4}$$

where

$$\boldsymbol{\Sigma}_r = \operatorname{diag}(r(x_0), r(x_1), \ldots, r(x_N)), \quad \boldsymbol{\Sigma}_s = \operatorname{diag}(s(x_0), s(x_1), \ldots, s(x_N)),$$
$$\boldsymbol{u} = (u_N(x_0), u_N(x_1), \ldots, u_N(x_N))^t, \quad \boldsymbol{f} = (f(x_0), f(x_1), \ldots, f(x_N))^t.$$

Using the new basis in (3.6), we write

$$u_N(x) = \sum_{j=0}^{N} v_j Q_j(x), \quad v_j := u_N''(x_j) - \nu^2 u_N(x_j).$$

Substituting it into (4.2), we obtain

$$-\sum_{j=0}^{N} v_j Q_j''(x_i) + r(x_i)\sum_{j=0}^{N} v_j Q_j'(x_i) + s(x_i)\sum_{j=0}^{N} v_j Q_j(x_i) = f(x_i), \quad 0 \le i \le N.$$

Then the matrix form of (4.2) reads

$$\left(-\boldsymbol{I}_{N+1} + \boldsymbol{\Sigma}_r \boldsymbol{Q}^{(1)} + (\boldsymbol{\Sigma}_s - \nu^2 \boldsymbol{I}_{N+1})\boldsymbol{Q}\right)\boldsymbol{v} = \boldsymbol{f}. \tag{4.5}$$

Remark 4.1. It is known that the resolution and accuracy of the spectral methods in unbounded domains can be enhanced by using a proper scaling parameter. For example, in actual computation, instead of solving (4.1), we solve the following scaled equation with the new variable $y = \beta x$:

$$-\beta^2 v''(y) + \beta a(y)v'(y) + b(y)v(y) = g(y), \quad y \in (-\infty, +\infty); \quad \lim_{|y|\to\infty} v(y) = 0, \tag{4.6}$$

where $v(y) = u(\beta x)$, $a(y) = r(\beta x)$, $b(y) = s(\beta x)$ and $g(y) = f(\beta x)$. The matrix system of the scaled problem (4.6) approximated by the new basis functions is

$$\left(-\beta^2 \boldsymbol{I}_{N+1} + \beta \boldsymbol{\Sigma}_r \boldsymbol{Q}^{(1)} + (\boldsymbol{\Sigma}_s - \beta^2\nu^2 \boldsymbol{I}_{N+1})\boldsymbol{Q}\right)\boldsymbol{v} = \boldsymbol{f}. \tag{4.7}$$

This also applies to the scheme in (4.4).

In the following test, we set $r(x) = 0$, $s(x) = x^2$ in (4.1), and choose the exact solution to be $u(x) = (1 + x^2)^{-5/2}$. In Table 4.1, we list the condition numbers of the schemes (4.4) and (4.5) with the scaling factor $\beta = 2$ and with $\nu = 1/2$ in (4.5). The results show that the condition numbers of the usual collocation scheme increase quickly as N increases, but these of the new collocation scheme are much smaller.

In Fig. 4.1, we plot the maximum point-wise errors of two schemes (4.4) and (4.5) with $\nu = 1/2$. And we observe that the new approach outperforms the usual method.

Similarly, we consider the model BVP on the half line:

$$-u''(x) + r(x)u'(x) + s(x)u(x) = f(x), \quad x \in (0, \infty); \quad u(0) = u_0, \quad \lim_{x\to\infty} u(x) = 0, \tag{4.8}$$

where the given functions $r, s, f \in C(\mathbb{R}^+)$.

Let $\{x_i\}_{i=0}^N$ be the LGR points as before. Then the collocation scheme for (4.8) is to find $u_N \in \widehat{\mathcal{P}}_N(\mathbb{R}^+)$ such that

$$\begin{cases} -u_N''(x_i) + r(x_i)u_N'(x_i) + s(x_i)u_N(x_i) = f(x_i), & 1 \le i \le N, \\ u_N(0) = u_0. \end{cases} \tag{4.9}$$

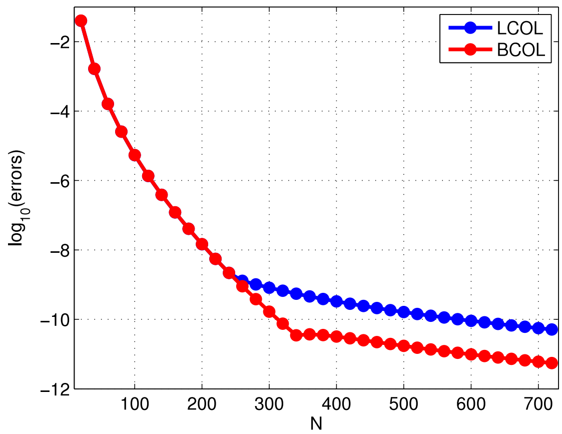

Fig. 4.1. Error plots: (4.4) (LCOL) versus (4.5) (BCOL).

(i) *Usual collocation scheme using Lagrange interpolating basis* (LCOL). Let $\{\hat{h}_j\}_{j=0}^N$ be the Lagrange interpolation functions defined in (2.26). We expand the numerical solution of (4.8) as

$$u_N(x) = u_0\hat{h}_0(x) + \sum_{j=1}^{N} u_N(x_j)\hat{h}_j(x),$$

and substitute it into (4.9), leading to

$$-\sum_{j=1}^{N} u_N(x_j)\hat{h}_j''(x_i) + r(x_i)\sum_{j=1}^{N} u_N(x_j)\hat{h}_j'(x_i) + s(x_i)\sum_{j=1}^{N} u_N(x_j)\hat{h}_j(x_i)$$
$$= f(x_i) + u_0\big(\hat{h}_0''(x_i) - r(x_i)\hat{h}_0'(x_i) - s(x_i)\hat{h}_0(x_i)\big), \quad 1 \le i \le N.$$

Thus, the above equations can be written in the form of matrix as follows:

$$\big(-\widehat{\boldsymbol{D}}_{\rm in}^{(2)} + \boldsymbol{\Sigma}_r\widehat{\boldsymbol{D}}_{\rm in}^{(1)} + \boldsymbol{\Sigma}_s\big)\,\boldsymbol{u} = \boldsymbol{f} + \boldsymbol{u}_B, \tag{4.10}$$

where

$$\boldsymbol{\Sigma}_r = \mathrm{diag}(r(x_1), r(x_2), \ldots, r(x_N)), \quad \boldsymbol{\Sigma}_s = \mathrm{diag}(s(x_1), s(x_2), \ldots, s(x_N)),$$
$$\boldsymbol{u} = (u_N(x_1), u_N(x_2), \ldots, u_N(x_N))^t, \quad \boldsymbol{f} = (f(x_1), f(x_2), \ldots, f(x_N))^t,$$

$\boldsymbol{u}_B$ is the vector of $\big\{u_0(\hat{d}_{i0}^{(2)} - r(x_i)\hat{d}_{i0}^{(1)})\big\}_{i=1}^N$.

(ii) *New collocation scheme using the new basis (BCOL).* Let $\{S_j\}$ be the new basis defined in (3.23) and write

$$u_N(x) = u_0S_0(x) + \sum_{j=1}^{N} v_jS_j(x), \quad v_j = u_N''(x_j) - \lambda^2u_N(x_j).$$

Substituting it into (4.9), we obtain

$$-\sum_{j=1}^{N} v_jS_j''(x_i) + r(x_i)\sum_{j=1}^{N} v_jS_j'(x_i) + s(x_i)\sum_{j=1}^{N} v_jS_j(x_i)$$
$$= f(x_i) + u_0S_0''(x_i) - r(x_i)u_0S_0'(x_i) - s(x_i)u_0S_0(x_i), \quad 1 \le i \le N.$$

Then the matrix form of (4.9) reads

$$\big(-\boldsymbol{I}_N + \boldsymbol{\Sigma}_r\boldsymbol{S}^{(1)} + (\boldsymbol{\Sigma}_s - \lambda^2\boldsymbol{I}_N)\boldsymbol{S}\big)\boldsymbol{v} = \boldsymbol{f} - u_0\boldsymbol{v}_-, \tag{4.11}$$

where $\boldsymbol{v}_-$ is vector with entries $\big\{r(x_i)S_0'(x_i) + (s(x_i) - \lambda^2)S_0(x_i)\big\}_{i=1}^N$.

Remark 4.2. Based on the new basis, a second collocation scheme is to precondition the collocation system (4.10) by using the matrix $\boldsymbol{S}$ in (3.17), that is,

$$\big(-\boldsymbol{S}(\widehat{\boldsymbol{D}}_{\rm in}^{(2)} - \lambda^2\boldsymbol{I}_N) + \boldsymbol{S}\,\boldsymbol{\Sigma}_r\widehat{\boldsymbol{D}}_{\rm in}^{(1)} + \boldsymbol{S}(\boldsymbol{\Sigma}_s - \lambda^2\boldsymbol{I}_N)\big)\,\boldsymbol{u} = \boldsymbol{S}(\boldsymbol{f} + \boldsymbol{u}_B). \tag{4.12}$$

Table 4.2
Condition numbers of two schemes with $\beta = 2$ and $\lambda = \frac{1}{2}$..

	$N = 100$	$N = 140$	$N = 180$	$N = 220$	$N = 260$
LCOL (4.10)	1.66E+03	3.24E+03	5.34E+03	7.96E+03	1.11E+04
BCOL (4.11)	8.82	10.4	11.8	13.2	14.6

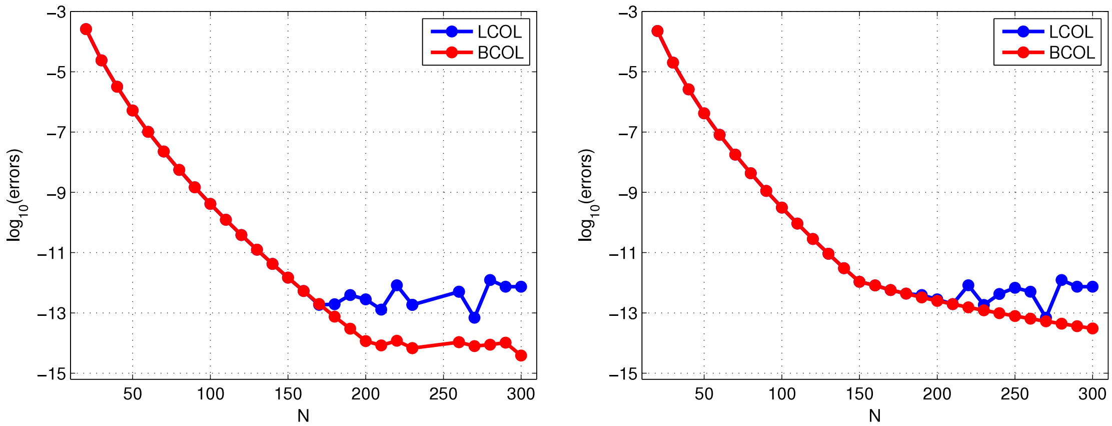

Fig. 4.2. Error behaviour of two schemes (4.10) and (4.11) with $\beta = 2$, $\lambda = 1/2$ and exact solutions: $u(x) = (1+x)^{-11/2}$ (left) and $u(x) = (\cos x)(1+x)^{-11/2}$ (right).

Note from Proposition 3.2 that $\boldsymbol{S}(\widehat{\boldsymbol{D}}_{\rm in}^{(2)} - \lambda^2 \boldsymbol{I}_N)$ is approximately an identity matrix. In particular, if $\lambda = 1/2$, we find from Proposition 3.3 that

$$\big(-\boldsymbol{I}_N + \boldsymbol{S}\,\boldsymbol{\Sigma}_r \widehat{\boldsymbol{D}}_{\rm in}^{(1)} + \boldsymbol{S}(\boldsymbol{\Sigma}_s - \boldsymbol{I}_N/4)\big)\,\boldsymbol{u} = \boldsymbol{S}(\boldsymbol{f} + \boldsymbol{u}_B). \tag{4.13}$$

In fact, the preconditioned approach has a performance very similar to that of (4.11), so hereafter, we just focus on the scheme (4.11).

Remark 4.3. As with Remark 4.1, we can introduce a scaling factor to enhance the resolution in a finite interval centred at the origin.

We next provide some numerical results to show the performance of the above schemes. Here, we take $r(x) = x$ and $s(x) = x^2$ in (4.8), and measure the maximum point-wise error: $\max_{0\le i\le N} |u(x_i) - u_N(x_i)|$. In Table 4.2, we compare the condition numbers of two schemes: (4.10) and (4.11) with the scaling factor $\beta = 2$ and with $\lambda = 1/2$ in (4.11). As expected, the condition numbers of the usual collocation scheme using polynomial basis increase quickly as N increases, which induces large round-off errors and numerical instability. In contrast, the new collocation scheme can overcome such a deficiency.

To show the accuracy and well conditioning of the linear system, we test the solutions: $u(x) = (1+x)^{-11/2}$ and $u(x) = (\cos x)(1+x)^{-11/2}$. In Fig. 4.2, we depict the numerical errors of two schemes, show that the new scheme does not suffer from the round-off errors, occurring in the usual collocation scheme for large N.

4.2. Two-dimensional case

Consider two-dimensional elliptic problem:

$$\Delta u - 2\nu^2 u = f, \quad (x, y) \in \mathbb{R}^2, \quad u(x, y) \to 0 \ \text{ as } \ |x|,\ |y| \to \infty, \tag{4.14}$$

where the function f is given. Let $\{(x_i, y_i)\}_{i,j=0}^N$ be the tensorial Hermite–Gauss points. Then the collocation scheme for (4.14) is to find $u_N \in \widehat{\mathcal{P}}_N(\mathbb{R}^2)$ such that

$$\Delta u_N(x_i, y_j) - 2\nu^2 u_N(x_i, y_j) = f(x_i, y_j), \quad 0 \le i, j \le N. \tag{4.15}$$

Using the new basis $\{Q_j\}$ with parameter $\nu > 0$, we can write

$$u_N(x, y) = \sum_{m,n=0}^{N} \bar{u}_{mn} Q_m(x) Q_n(y).$$

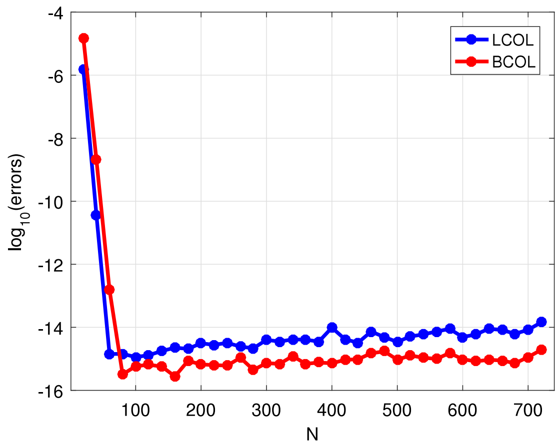

Fig. 4.3. The new scheme versus the usual collocation method for two-dimensional example (4.14).

Note that by (3.2),

$$\Delta u_N - 2\nu^2 u_N = \sum_{m,n=0}^{N} \bar{u}_{mn} h_m(x) Q_n(y) + \sum_{m,n=0}^{N} \bar{u}_{mn} Q_m(x) h_n(y).$$

Thus, (4.15) becomes the following linear system:

$$\boldsymbol{U}\boldsymbol{Q}^t + \boldsymbol{Q}\boldsymbol{U} = \boldsymbol{F}, \tag{4.16}$$

where $\boldsymbol{U} = (\bar{u}_{mn})_{m,n=0,\ldots,N}$ and $\boldsymbol{F} = (f(x_i, y_j))_{i,j=0,\ldots,N}$.

Similarly, we can formulate the two-dimensional tensorial version of the usual collocation scheme (LCOL) (cf. [6]).

We take the test solution $u(x, y) = e^{-(x^2+y^2)} \sin x \sin y$. In Fig. 4.3, we plot the maximum pointwise errors with $\nu = 1$ of the new scheme (BCOL) and LCOL for various N. Once again, we observe that the BCOL has smaller round-off errors than LCOL for large N.

4.3. Applications to time-dependent problems

As an example, we consider the application of the new collocation scheme in spatial discretization of the Burger's equation on the half line:

$$\begin{cases} \partial_t u + u\partial_x u = \nu \partial_x^2 u + f, & x \in \mathbb{R}^+, \quad t \in (0, T], \\ u(0, t) = v_-(t), \quad \lim_{x\to\infty} u(x, t) = 0, & t \in (0, T], \\ u(x, 0) = u_0(x), & x \in \mathbb{R}^+, \end{cases} \tag{4.17}$$

where ν is a positive constant, and v_-, u_0 are given.

Let τ be the mesh size in time t and $t_n = n\tau$ for $n = 0, 1, \ldots$. We employ the second-order Crank–Nicolson scheme with spatial discretization by the new basis $\{S_j\}$ (with $\lambda = 1/\sqrt{\nu\tau}$) for (4.17), that is, to find the approximation of $u(x, t_n)$ as

$$u_N^n(x) = v_-(t_n) S_0(x) + \sum_{j=1}^{N} v_j^n S_j(x), \quad n \geq 0, \tag{4.18}$$

such that

$$\frac{u_N^{n+1}(x_i) - u_N^{n-1}(x_i)}{2\tau} + u_N^n(x_i)\partial_x u_N^n(x_i) = \nu \partial_x^2 \Big(\frac{u_N^{n+1} + u_N^{n-1}}{2}\Big)(x_i) + f(t_n, x_i), \tag{4.19}$$

for $1 \leq i \leq N$ and $n \geq 1$.

Inserting the above expansion (4.18) into (4.19), we have from (3.18) (with $\lambda = 1/\sqrt{\nu\tau}$) that

$$\boldsymbol{v}^{n+1} = -(2\lambda^2 \boldsymbol{S} + \boldsymbol{I}_N)\boldsymbol{v}^{n-1} - 2\lambda^2 v_-(t_{n-1}) S_0(x_i) + \frac{2}{\nu}\boldsymbol{F}^n, \quad n \geq 1, \tag{4.20}$$

where

$$\boldsymbol{v}^n = (v_1^n, v_2^n, \ldots, v_N^n)^t, \quad \boldsymbol{F}^n = (f_1^n, f_2^n, \ldots, f_N^n)^t, \quad f_i^n = u_N^n(x_i)\partial_x u_N^n(x_i) - f(t_n, x_i).$$

Similarly, we can formula the usual collocation scheme using Lagrange basis functions (LCOL). Here, we omit the details.

Table 4.3
Comparison of CPU time, errors and order in time.

τ	LCOL			BCOL		
	CPU (s)	Error	Order	CPU (s)	Error	Order
0.0100	20.78	1.39E−05	–	6.68	1.39E−05	–
0.0050	41.00	3.47E−06	2.0021	11.39	3.47E−06	2.0021
0.0010	201.81	1.39E−07	1.9991	47.75	1.39E−07	1.9991
0.0005	397.65	3.47E−08	2.0021	93.60	3.44E−08	2.0146

We consider (4.17) with $T = 30$, $\nu = 0.01$, and take the test solution: $u(x, t) = e^{-x} \sin x \sin t$. In Table 4.3, we compared the CPU times and maximum point-wise errors at the final time T using LCOL scheme and the new scheme (BCOL) with $N = 350$. The results show that both schemes have the second order convergence accuracy. Although the maximum point-wise errors of the two schemes are almost the same, the new scheme is much faster for small time-stepping size than the LCOL scheme.

4.4. A composite Legendre–Laguerre collocation scheme

To further demonstrate the advantage of the new approach, we glue it with the Legendre–Birkhoff collocation method introduced in [22] for problems in unbounded domains. This domain decomposition method can significantly enhance the accuracy as the Legendre approximation has a much better resolution over a finite interval. Indeed, the composite Legendre–Laguerre Galerkin method outperformed the pure Laguerre–Galerkin approach [47]. However, there appears no discussion on the composite collocation method posed on the strong form of a differential equation.

To fix the idea, we consider the boundary value problem:

$$\begin{cases} -u''(x) + r(x)u'(x) + s(x)u(x) = f(x), & x \in \Omega := (-2, \infty), \\ u(-2) = u_-, \quad \lim_{x\to\infty} u(x) = 0, \end{cases} \tag{4.21}$$

where the given functions $r, s, f \in C(\Omega)$, and u_- is a given number.

We decompose the domain into $\Omega = \bar{I} \cup \mathbb{R}^+$ with $I := (-2, 0)$. Let $\{\xi_j\}_{j=0}^{L} \subseteq [-1, 1]$ with $\xi_0 = -1$ and $\xi_L = 1$ be the Legendre–Gauss–Lobatto (LGL) points, and $\{x_j\}_{j=0}^{N}$ be Laguerre–Gauss–Radau points as before. Define the approximation space

$$X_N^L = \left\{ v \in C^1(\Omega) : v|_I \in \mathcal{P}_L \text{ and } v|_{\mathbb{R}^+} \in \widehat{\mathcal{P}}_N(\mathbb{R}^+) \right\},$$

where $\mathcal{P}_L$ is the set of all polynomials of degree not more than L, and $\widehat{\mathcal{P}}_N(\mathbb{R}^+)$ is defined in (2.24). Note that $\dim(X_N^L) = L+N$. The approximate solution $U_* \in X_N^L$ consists of two pieces:

$$U_*(x) = \begin{cases} U_{l,*} \in \mathcal{P}_L, & x \in I, \\ U_{r,*} \in \widehat{\mathcal{P}}_N(\mathbb{R}^+), & x \in \mathbb{R}^+, \end{cases} \text{ such that } [\![U_*]\!](0) = [\![U_*']\!](0) = 0, \tag{4.22}$$

where $[\![\cdot]\!](0)$ stands for the jump at $x = 0$. It is determined by the composite collocation scheme:

$$\begin{cases} -U_{l,*}''(y_j) + r(y_j)U_{l,*}'(y_j) + s(y_j)U_{l,*}(y_j) = f(y_j), & 1 \le j \le L-1, \\ -U_{r,*}''(x_j) + r(x_j)U_{r,*}'(x_j) + s(x_j)U_{r,*}(x_j) = f(x_j), & 1 \le j \le N, \\ U_{l,*}(y_0) = u_-; \quad [\![U_*]\!](0) = [\![U_*']\!](0) = 0, \end{cases} \tag{4.23}$$

where $y_j = \xi_j - 1$.

We now introduce the basis functions of X_N^L. On the finite interval, we shall use the Legendre–Birkhoff interpolating basis polynomials introduced in [22] through Birkhoff interpolation. More precisely, the basis $\{B_j\}_{j=0}^{L} \subseteq \mathcal{P}_L$ with $\xi \in (-1, 1)$ satisfies

$$B_0(-1) = 1, \quad B_0(1) = 0, \quad B_0''(\xi_i) = 0, \quad 1 \le i \le L-1; \tag{4.24}$$

$$B_j(-1) = 0, \quad B_j(1) = 0, \quad B_j''(\xi_i) = \delta_{ij}, \quad 1 \le i, j \le L-1; \tag{4.25}$$

$$B_L(-1) = 0, \quad B_L(1) = 1, \quad B_L''(\xi_i) = 0, \quad 1 \le i \le L-1. \tag{4.26}$$

We refer to [22] for the expressions and calculation of $\{B_j\}$.

For the Laguerre approximation, we use the new basis $\{S_j\}_{j=0}^{N}$ with $\lambda = 1/2$, so $S_0(x) = e^{-x/2}$ and $\{S_j\}_{j=1}^{N}$ are defined in (3.31). Define

$$\Phi_j(x) = \begin{cases} B_j(\xi), & x \in I, \\ 0, & x \in \mathbb{R}^+, \end{cases} \quad \Phi_k(x) = \begin{cases} S_{k-L}(x), & x \in \mathbb{R}^+, \\ 0, & x \in I, \end{cases} \quad \Phi_L(x) = \begin{cases} B_L(\xi), & x \in I, \\ S_0(x), & x \in \mathbb{R}^+, \end{cases} \tag{4.27}$$

for $0 \le j \le L-1$, $L+1 \le k \le L+N$, and $\xi = x + 1$. Write

$$U_*(x) = u_- \Phi_0(x) + \sum_{k=1}^{L+N} \hat{u}_k \Phi_k(x), \tag{4.28}$$

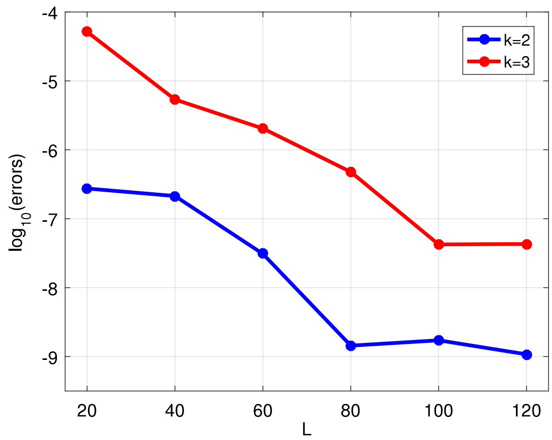

Fig. 4.4. Errors with $\lambda = 1/2$ and $N = 2L$.

which implies $U_* \in C(\Omega)$, so $[\![U_*]\!](0) = 0$. We impose $[\![U'_*]\!](0) = 0$ directly, leading to

$$-\frac{u_-}{2} + \sum_{k=1}^{L-1} \hat{u}_k B'_k(1) + \frac{\hat{u}_L}{2} = -\frac{\hat{u}_L}{2} + \sum_{k=L+1}^{L+N} \hat{u}_k S'_{k-L}(0). \tag{4.29}$$

Then substituting (4.28) into the scheme (4.23), we can obtain the linear system straightforwardly. Again, we are able to take the advantage of using this set of basis functions, that is, in the two sub-matrices on the main diagonal block, the contributions from the second-order derivatives are diagonal. In other words, the two sub-matrices are well-conditioned, so the system can be solved efficiently and stably even for large L, N.

We solve the problem (4.21) with $r(x) = x$, $s(x) = x^2$, and take the test function $u(x) = (\cos kx)(3+x)^{-11/2}$, which decays algebraically as x goes to infinity. In Fig. 4.4, we plot the maximum point-wise errors with $\lambda = 1/2$ and $N = 2L$ v.s. the modes L. The numerical results demonstrate the convergence of the method with L. The numerical errors show the high accuracy of the proposed algorithm. The results also indicate that the smoother the exact solution, the better the numerical results.

4.5. Concluding remarks

In this paper, we constructed two sets of non-standard basis functions for Hermite/Laguerre collocation methods. Fast and stable algorithms for the basis functions were provided. In addition, we demonstrated that the new basis functions have the good approximability to the Laguerre/Hermite orthogonal functions. Using the new basis functions, we proposed new collocation schemes for general second-order boundary value problems with (i) the matrix corresponding to the operators being identity; (ii) the linear systems being well-conditioned. Numerical results for various problems indicated the efficiency and high accuracy of the proposed new approaches.

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