

Spectral Method for Unbounded Domains

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1 Laguerre Polynomials/Functions

1.1 (Generalized) Laguerre Polynomials

- Laguerre polynomials, denoted by $\mathcal{L}_n(x)$, are orthogonal w.r.t. $\omega(x) = e^{-x}$, on the half line $\mathbb{R}_+ := (0, +\infty)$, i.e.

$$\int_0^{+\infty} \mathcal{L}_n(x) \mathcal{L}_m(x) e^{-x} dx = \delta_{mn}. \quad (1)$$

- The Generalized Laguerre polynomials (GLPs), denoted by $\mathcal{L}_n^{(\alpha)}(x)$, $\alpha > -1$ are orthongal w.r.t. $\omega_\alpha(x) = x^\alpha e^{-x}$ on $\mathbb{R}_+$, i.e.

$$\int_0^{+\infty} \mathcal{L}_n(x) \mathcal{L}_m(x) \omega_\alpha(x) dx = \gamma_n^{(\alpha)} \delta_{mn}, \quad (2)$$

where

$$\gamma_n^{(\alpha)} = \frac{\Gamma(n + \alpha + 1)}{n!}. \quad (3)$$

Basic properties of GLPs

1. Three-term recurrence formula

$$(n+1)\mathcal{L}_{n+1}^{(\alpha)}(x) = (2n+\alpha+1-x)\mathcal{L}_n^{(\alpha)}(x) - (n+\alpha)\mathcal{L}_{n-1}^{(\alpha)}(x),$$

$$\mathcal{L}_0^{(\alpha)}(x) = 1, \quad \mathcal{L}_1^{(\alpha)}(x) = -x + \alpha + 1.$$

2. Leading coefficient: $k_n^{(\alpha)} = \frac{(-1)^n}{n!}$,

value at 0: $\mathcal{L}_n^{(\alpha)}(0) = \frac{\Gamma(n+\alpha+1)}{n!\Gamma(\alpha+1)}$

3. Sturm–Liouville equation ($\lambda_n = n$!)

$$x^{-\alpha} e^x \partial_x \left(x^{\alpha+1} e^{-x} \partial_x \mathcal{L}_n^{(\alpha)}(x) \right) + \lambda_n \mathcal{L}_n^{(\alpha)}(x) = 0, \quad (4)$$

$$x \partial_x^2 \mathcal{L}_n^{(\alpha)}(x) + (\alpha + 1 - x) \partial_x \mathcal{L}_n^{(\alpha)}(x) + \lambda_n \mathcal{L}_n^{(\alpha)}(x) = 0. \quad (5)$$

4. $\left\{ \partial_x \mathcal{L}_n^{(\alpha)} \right\}$ orthogonal w.r.t. $\omega_{\alpha+1}$

$$\int_0^{+\infty} \partial_x \mathcal{L}_n^{(\alpha)}(x) \partial_x \mathcal{L}_m^{(\alpha)}(x) \omega_{\alpha+1}(x) dx = \lambda_n \gamma_n^{(\alpha)} \delta_{mn}. \quad (6)$$

5. Rodrigues's formula

$$\mathcal{L}_n^{(\alpha)}(x) = \frac{x^{-\alpha} e^x}{n!} \frac{d^n}{dx^n} \{x^{n+\alpha} e^{-x}\}. \quad (7)$$

Explicit expression

$$\mathcal{L}_n^{(\alpha)}(x) = \sum_{k=0}^n \frac{(-1)^k}{k!} \binom{n+\alpha}{n-k} x^k$$

6. Derivatives

$$\begin{aligned} \partial_x \mathcal{L}_n^{(\alpha)}(x) &= -\mathcal{L}_{n-1}^{(\alpha+1)}(x) = -\sum_{k=0}^{n-1} \mathcal{L}_k^{(\alpha)}(x), \\ \mathcal{L}_n^{(\alpha)}(x) &= \partial_x \mathcal{L}_n^{(\alpha)}(x) - \partial_x \mathcal{L}_{n+1}^{(\alpha)}(x), \\ x \partial_x \mathcal{L}_n^{(\alpha)}(x) &= n \mathcal{L}_n^{(\alpha)}(x) - (n+\alpha) \mathcal{L}_{n-1}^{(\alpha)}(x), \end{aligned} \quad (8)$$

7. Asymptotic properties of the GLPs.

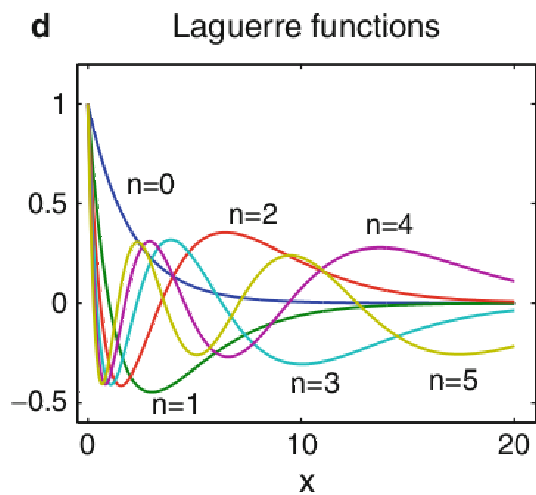
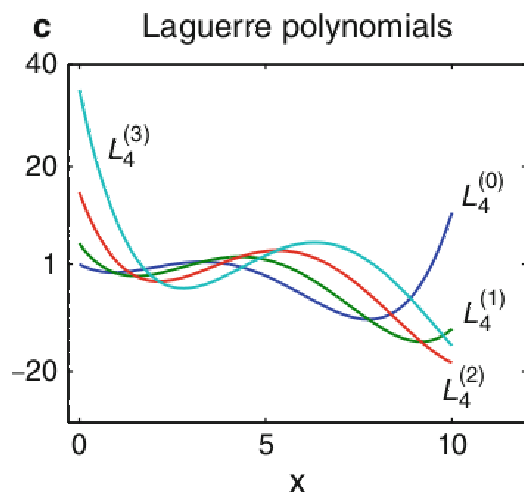
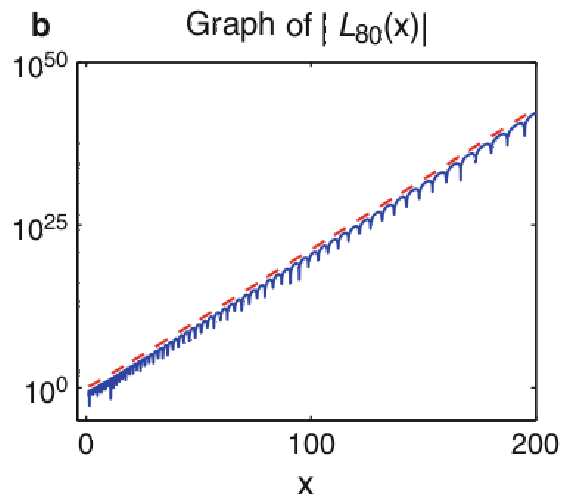
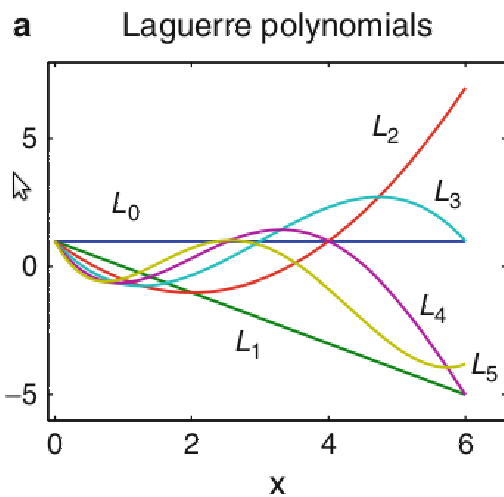
- For large x , $\mathcal{L}_n^{(\alpha)}(x)$ is dominated by leading term $\frac{(-1)^n}{n!}x^n$
- Theorem 8.22.5 of Szegö (1975)

$$\mathcal{L}_n^{(\alpha)}(x) = \sqrt{\frac{n^{\alpha - \frac{1}{2}} e^x}{\pi x^{\alpha + \frac{1}{2}}}} \left[\cos \left(2\sqrt{nx} - \frac{2\alpha + 1}{4}\pi \right) + \frac{O(1)}{\sqrt{nx}} \right] \quad (9)$$

for all $x \in [c/n, b]$.

- upper bounds

$$\left| \mathcal{L}_n^{(\alpha)}(x) \right| \leq \begin{cases} \mathcal{L}_n^{(\alpha)}(0) e^{x/2}, & \text{if } \alpha \geq 0, \\ \left(2 - \mathcal{L}_n^{(\alpha)}(0) \right) e^{x/2}, & \text{if } \alpha < 0. \end{cases} \quad (10)$$



1.2 Generalized Laguerre Functions (GLFs)

Definition:

$$\hat{\mathcal{L}}_n^{(\alpha)}(x) := e^{-x/2} \mathcal{L}_n^{(\alpha)}(x), \quad x \in \mathbb{R}_+, \quad \alpha > -1.$$

GLFs are orthogonal w.r.t weight function $\hat{\omega}_\alpha = x^\alpha$, i.e.

$$\int_0^{+\infty} \hat{\mathcal{L}}_n^{(\alpha)}(x) \hat{\mathcal{L}}_m^{(\alpha)}(x) \hat{\omega}_\alpha(x) dx = \gamma_n^{(\alpha)} \delta_{nm}. \quad (11)$$

Introducing

$$\hat{\partial}_x = \partial_x + \frac{1}{2} \quad (12)$$

then

$$\partial_x \mathcal{L}_n^{(\alpha)}(x) = e^{x/2} \hat{\partial}_x \hat{\mathcal{L}}_n^{(\alpha)}(x). \quad (13)$$

Basic properties of GLFs

- Three-term recurrence relation

$$(n+1)\hat{\mathcal{L}}_{n+1}^{(\alpha)}(x) = (2n+\alpha+1-x)\hat{\mathcal{L}}_n^{(\alpha)}(x) - (n+\alpha)\hat{\mathcal{L}}_{n-1}^{(\alpha)}(x),$$

$$\hat{\mathcal{L}}_0^{(\alpha)}(x) = e^{-x/2}, \quad \hat{\mathcal{L}}_1^{(\alpha)}(x) = (\alpha+1-x)e^{-x/2}.$$

- Decay property

$$\left| \hat{\mathcal{L}}_n^{(\alpha)}(x) \right| \rightarrow 0, \quad x \rightarrow +\infty \quad (14)$$

$$\left| \hat{\mathcal{L}}_n^{(\alpha)}(x) \right| \leq 1, \quad \forall x \in [0, +\infty) \quad (15)$$

- Sturm–Liouville equation

$$x^{-\alpha}e^{x/2}\partial_x\left(x^{\alpha+1}e^{-x/2}\hat{\partial}_x\hat{\mathcal{L}}_n^{(\alpha)}(x)\right) + n\hat{\mathcal{L}}_n^{(\alpha)}(x) = 0. \quad (16)$$

- Orthogonality

$$\int_0^{+\infty} \hat{\partial}_x \hat{\mathcal{L}}_n^{(\alpha)}(x) \hat{\partial}_x \hat{\mathcal{L}}_m^{(\alpha)}(x) \hat{\omega}_{\alpha+1}(x) dx = \lambda_n \gamma_n^{(\alpha)} \delta_{mn}. \quad (17)$$

- Derivative relation

$$\begin{aligned} \hat{\partial}_x \hat{\mathcal{L}}_n^{(\alpha)}(x) &= -\hat{\mathcal{L}}_{n-1}^{(\alpha+1)}(x) = -\sum_{k=0}^{n-1} \hat{\mathcal{L}}_k^{(\alpha)}(x), \\ \hat{\mathcal{L}}_n^{(\alpha)}(x) &= \hat{\partial}_x \hat{\mathcal{L}}_n^{(\alpha)}(x) - \hat{\partial}_x \hat{\mathcal{L}}_{n+1}^{(\alpha)}(x), \\ x \hat{\partial}_x \hat{\mathcal{L}}_n^{(\alpha)}(x) &= n \hat{\mathcal{L}}_n^{(\alpha)}(x) - (n + \alpha) \hat{\mathcal{L}}_{n-1}^{(\alpha)}(x), \end{aligned} \quad (18)$$

1.3 Laguerre–Gauss Type Quadarature

Theorem 1. Let $\{x_j^\alpha, \omega_j^\alpha\}_{j=0}^N$ be the set of LG or LGR nodes and weights.

- *Laguerre–Gauss (LG):* $\{x_j^\alpha\}_{j=0}^N$ are zeros of $\mathcal{L}_{N+1}^{(\alpha)}(x)$,

$$\begin{aligned}\omega_j^\alpha &= -\frac{\Gamma(N+\alpha+1)}{(N+1)!} \frac{1}{\mathcal{L}_N^{(\alpha)}(x_j^\alpha) \partial_x \mathcal{L}_{N+1}^{(\alpha)}(x_j^\alpha)} \\ &= \frac{\Gamma(N+\alpha+1)}{(N+\alpha+1)(N+1)!} \frac{x_j^\alpha}{\left[\mathcal{L}_N^{(\alpha)}(x_j^\alpha)\right]^2}, \quad 0 \leq j \leq N.\end{aligned}\tag{19}$$

- *Laguerre–Gauss–Radau (LGR):* $x_0^\alpha = 0$ and $\{x_j^\alpha\}_{j=1}^N$ are zeros of $\partial_x \mathcal{L}_{N+1}^{(\alpha)}(x)$;

$$\begin{aligned}\omega_0^\alpha &= \frac{(\alpha+1)\Gamma^2(\alpha+1)N!}{\Gamma(N+\alpha+2)}, \quad \omega_j^\alpha = \frac{\Gamma(N+\alpha+1)}{N!(N+\alpha+1)} \frac{1}{\left[\partial_x \mathcal{L}_N^{(\alpha)}(x_j^\alpha)\right]^2} \\ &= \frac{\Gamma(N+\alpha+1)}{N!(N+\alpha+1)} \frac{1}{\left[\mathcal{L}_N^{(\alpha)}(x_j^\alpha)\right]^2}, \quad 1 \leq j < N.\end{aligned}\tag{20}$$

with $\delta = 1, 0$ for LG and LGR quadrature, respectively, we have

$$\int_0^{+\infty} p(x) x^\alpha e^{-x} dx = \sum_{j=0}^N p(x_j^\alpha) \omega_j^\alpha, \quad \forall p \in P_{2N+\delta},\tag{21}$$

Remark 2. Denote $\{x_j, \omega_j\}_{j=0}^N$ the usual ($\alpha = 0$) Laguerre–Gauss type nodes and weights

- LG case: $\{x_j\}_{j=0}^N$ zeros of $\mathcal{L}_{N+1}(x)$,

$$\omega_j = \frac{x_j}{(N+1)\mathcal{L}_N^2(x_j)}, \quad 0 \leq j \leq N. \quad (22)$$

- LGR case: $x_0 = 0$, $\{x_j\}_{j=1}^N$ zeros of $\partial_x \mathcal{L}_{N+1}(x)$,

$$\omega_j = \frac{1}{(N+1)\mathcal{L}_N^2(x_j)}, \quad 0 \leq j \leq N. \quad (23)$$

We find from (9) that weights are exponentially small for large x_j .

$$\mathcal{L}_N(x) \sim e^{x/2}(Nx)^{-1/4} \implies \omega_j \sim e^{-x_j} \sqrt{\frac{x_j}{N}}$$

Theorem 3. Let $\{x_j^\alpha, \omega_j^\alpha\}_{j=0}^N$ be the LG or LGR quadrature nodes and weights. Define

$$\hat{\omega}_j^\alpha = e^{x_j^\alpha} \omega_j^\alpha, \quad 0 \leq j \leq N, \quad (24)$$

and

$$\hat{P}_N := \{ \phi: \phi = e^{-x/2} \psi, \quad \forall \psi \in P_N \}. \quad (25)$$

Then we have the *modified quadrature formula*

$$\int_0^{+\infty} p(x) x^\alpha dx = \sum_{j=0}^N p(x_j^\alpha) \hat{\omega}_j^\alpha, \quad \forall p \in \hat{P}_{2N+\delta}, \quad (26)$$

where $\delta = 1, 0$ for the modified Laguerre–Gauss rule and the modified Laguerre–Gauss–Radau rule, respectively.

Remark 4. For $\alpha = 0$, $\hat{\omega}_j = \frac{1}{(N+1)[\hat{\mathcal{L}}_N(x_j)]^2}$, $0 \leq j \leq N \implies \hat{\omega}_j = O(\sqrt{x_j/N})$.

Computation of Nodes and Weights

- Eigenvalue method to calculate the nodes $\{x_j^\alpha\}_{j=0}^N$

$$A_{N+1} = \begin{pmatrix} a_0 & -\sqrt{b_1} & & & \\ -\sqrt{b_1} & a_1 & -\sqrt{b_2} & & \\ & \ddots & \ddots & \ddots & \\ & & -\sqrt{b_{N-1}} & a_{N-1} & -\sqrt{b_N} \\ & & & -\sqrt{b_N} & a_N \end{pmatrix},$$

$$a_j = 2j + \alpha + 1, \quad 0 \leq j \leq N; \quad b_j = j(j + \alpha), \quad 1 \leq j \leq N.$$

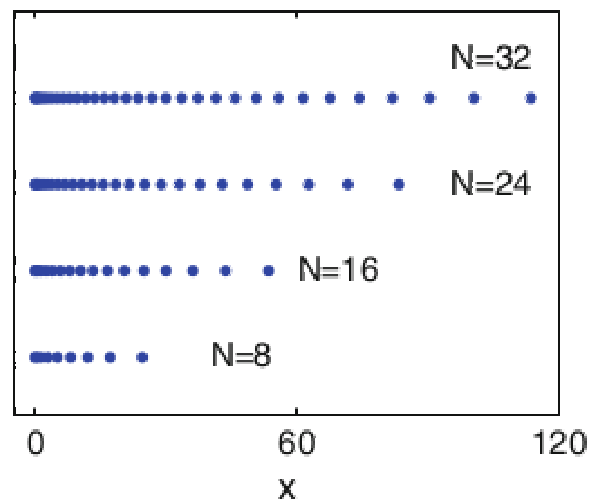
- First calculate weights $\{\hat{\omega}_j^\alpha\}_{j=0}^N$, then compute $\{\omega_j^\alpha\}_{j=0}^N$ by

$$\omega_j^\alpha = e^{-x_j^\alpha} \hat{\omega}_j^\alpha, \quad 0 \leq j \leq N.$$

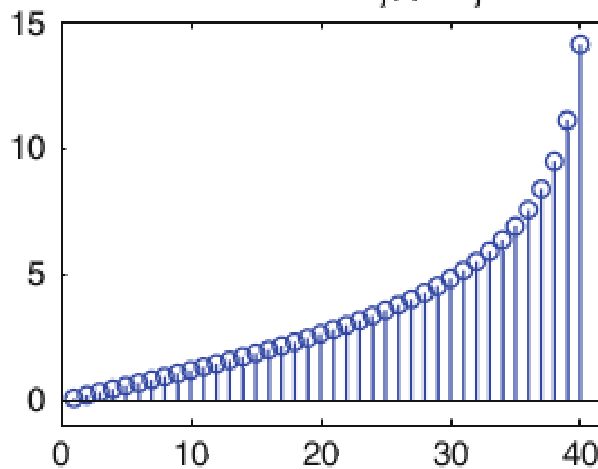
- Nodes distribution:

$$\min_j \{x_j^\alpha\} \sim N^{-1}, \max_j \{x_j^\alpha\} \sim 4N, \min_j |x_{j+1}^\alpha - x_j^\alpha| \sim N^{-1}$$

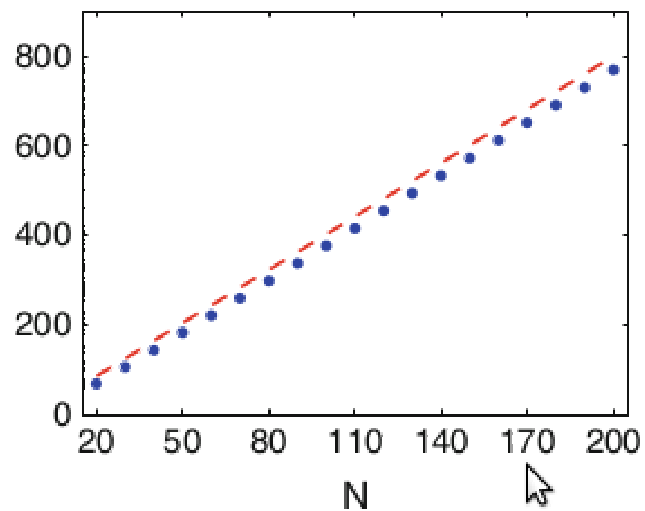
a Node distribution



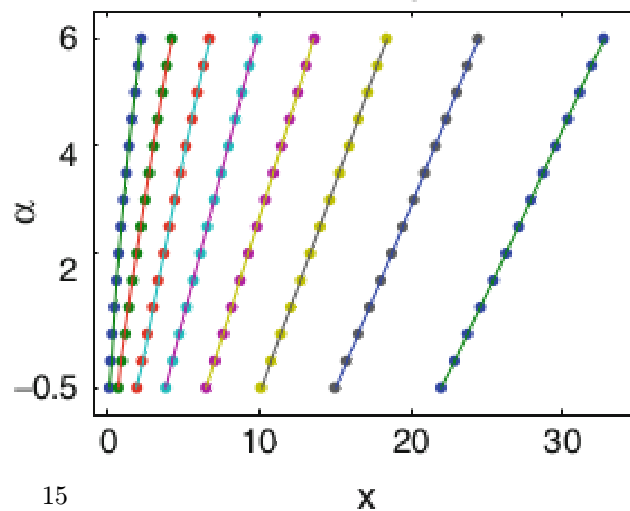
b Growth of $|x_{j+1} - x_j|$



c Growth of the largest node



d Zeros of $L_8^{(\alpha)}(x)$



1.4 Interpolation and Discrete Laguerre Transform

$\{x_j^\alpha, \hat{\omega}_j^\alpha\}_{j=0}^N$ modified LG or LGR nodes and weights, define

$$\langle u, v \rangle_{N, \hat{\omega}_\alpha} = \sum_{j=0}^N u(x_j^\alpha) v(x_j^\alpha) \hat{\omega}_j^\alpha, \quad \|u\|_{N, \hat{\omega}_\alpha} = \sqrt{\langle u, u \rangle_{N, \hat{\omega}_\alpha}}.$$

The exactness of the Gauss quadrature implies

$$\langle p, q \rangle_{N, \hat{\omega}_\alpha} = (p, q)_{\hat{\omega}_\alpha}, \quad \forall p, q \in \hat{P}_{2N+\delta}, \quad (27)$$

where $\delta = 1, 0$ for the modified LG and LGR quadrature, respectively.

Define **interpolation** $\hat{I}_N^{(\alpha)}: C[0, +\infty) \rightarrow \hat{P}_N$ as

$$\left(\hat{I}_N^{(\alpha)} u \right)(x) = \sum_{n=0}^N \tilde{u}_n^\alpha \hat{\mathcal{L}}_n^{(\alpha)}(x).$$

such that

$$\left(\hat{I}_N^{(\alpha)} u \right)(x_j^\alpha) = u(x_j^\alpha), \quad 0 \leq j \leq N.$$

Given the physical values $\{u(x_j^\alpha)\}_{j=0}^N$, the coefficients $\{\tilde{u}_n^\alpha\}_{n=0}^N$ can be determined by the **forward discrete transform**:

$$\tilde{u}_n^\alpha = \frac{1}{\gamma_n^{(\alpha)}} \sum_{j=0}^N u(x_j^\alpha) \hat{\mathcal{L}}_n^{(\alpha)}(x_j^\alpha) \hat{\omega}_j^\alpha, \quad 0 \leq n \leq N.$$

Backward discrete transform calculates $\{u(x_j^\alpha)\}_{j=0}^N$ using $\{\tilde{u}_n^\alpha\}_{n=0}^N$:

$$u(x_j^\alpha) = \sum_{n=0}^N \tilde{u}_n^\alpha \hat{\mathcal{L}}_n^{(\alpha)}(x_j^\alpha), \quad 0 \leq j \leq N.$$

The above definitions extends to usual Laguerre-Gauss transform directly (by removing “ $\wedge$ ”).

1.5 Differentiation

Differentiation in Physical Space

- Differentiation in Laguerre polynomials space P_N :
 $\{h_j\}$ Lagrange polynomials assoc. with LGR points $\{x_j^\alpha\}_{j=0}^N$.
 $u \in P_N$, $\mathbf{u}^{(m)} = (u^{(m)}(x_0^\alpha), \dots, u^{(m)}(x_N^\alpha))^T$, $\mathbf{u} := \mathbf{u}^{(0)}$, then

$$\mathbf{u}^{(m)} = D^m \mathbf{u}, \quad m \geq 1, \quad (28)$$

where $D = (d_{kj})_{k,j=0,\dots,N}$, $d_{kj} = h_j'(x_k)$.

- Differentiation in Laguerre function space $\hat{P}_N$:

$$\hat{h}_j(x) = e^{-x/2} / e^{-x_j^\alpha/2} h_j(x). \quad (29)$$

then

$$\hat{h}_j(x_k^\alpha) = \delta_{kj}, \quad 0 \leq k, j \leq N; \quad \hat{P}_N = \text{span}\{\hat{h}_j : 0 \leq j \leq N\}.$$

Moreover $\hat{h}_j' \in \hat{P}_N$ and

$$\hat{d}_{kj} := \hat{h}_j'(x_k^\alpha) = e^{-x_k^\alpha/2} / e^{-x_j^\alpha/2} d_{kj} - \frac{1}{2} \delta_{kj}, \quad 0 \leq j, k \leq N. \quad (30)$$

Differentiation in spectral space

$$u(x) = \sum_{n=0}^N \hat{u}_n \mathcal{L}_n^{(\alpha)}(x), \quad \hat{u}_n = \frac{1}{\gamma_n^{(\alpha)}} \int_0^{+\infty} u(x) \mathcal{L}_n^{(\alpha)}(x) \omega_\alpha(x) dx,$$

$$u'(x) = \sum_{n=1}^N \hat{u}_n \partial_x \mathcal{L}_n^{(\alpha)}(x) = \sum_{n=0}^N \hat{u}_n^{(1)} \mathcal{L}_n^{(\alpha)}(x) \in P_{N-1}, \quad \hat{u}_N^{(1)} = 0.$$

The coefficients $\{\hat{u}_n^{(1)}\}_{n=0}^{N-1}$ can be calculated from $\{\hat{u}_n\}_{n=1}^N$ by

$$\begin{cases} \hat{u}_{n-1}^{(1)} = \hat{u}_n^{(1)} - \hat{u}_n, & n = N, N-1, \dots, 1, \\ \hat{u}_N^{(1)} = 0. \end{cases} \quad (31)$$

Similarly, for the Laguerre function case (in space $\hat{P}_N$)

$$\begin{cases} \hat{v}_n^{(1)} = \hat{v}_{n+1}^{(1)} - \frac{1}{2}(\hat{v}_n + \hat{v}_{n+1}), & n = N-1, \dots, 0, \\ \hat{v}_N^{(1)} = -\frac{1}{2}\hat{v}_N. \end{cases} \quad (32)$$

2 Hermite Polynomials/Functions

2.1 Hermite polynomials

1. $H_m(x)$ defined on $\mathbb{R} := (-\infty, +\infty)$, weight $\omega(x) = e^{-x^2}$

$$\int_{-\infty}^{\infty} H_m(x) H_n(x) \omega(x) dx = \gamma_n \delta_{mn}, \quad \gamma_n = \sqrt{\pi} 2^n n!. \quad (33)$$

2. Three-term recurrence relation

$$H_{n+1}(x) = 2x H_n(x) - 2n H_{n-1}(x), \quad n \geq 1, \quad (34)$$

$$H_0(x) = 1, \quad H_1(x) = 2x.$$

Leading coefficient $k_n = 2^n$.

3. Connection with Laguerre polynomials

$$\begin{aligned} H_{2n}(x) &= (-1)^n 2^{2n} n! \mathcal{L}_n^{(-1/2)}(x^2), \\ H_{2n+1}(x) &= (-1)^n 2^{2n+1} n! x \mathcal{L}_n^{(1/2)}(x^2). \end{aligned} \quad (35)$$

4. Values at 0:

$$H_{2n}(0) = (-2)^n (2n-1)!!, \quad H_{2n+1}(0) = 0. \quad (36)$$

5. Sturm–Liouville equation:

$$e^{x^2} (e^{-x^2} H'_n(x))' + \lambda_n H_n(x) = 0, \quad \lambda_n = 2n, \quad (37)$$

$$H''_n(x) - 2x H'_n(x) + \lambda_n H_n(x) = 0. \quad (38)$$

6. Rodrigues' formula

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} \{e^{-x^2}\}, \quad (39)$$

explicit expression

$$H_n(x) = \sum_{k=0}^{[n/2]} \frac{(-1)^k n!}{k! (n-2k)!} (2x)^{n-2k}. \quad (40)$$

7. Upper bound

$$|H_n(x)| < c 2^{n/2} \sqrt{n!} e^{x^2/2}, \quad c \approx 1.086435. \quad (41)$$

8. Derivatives

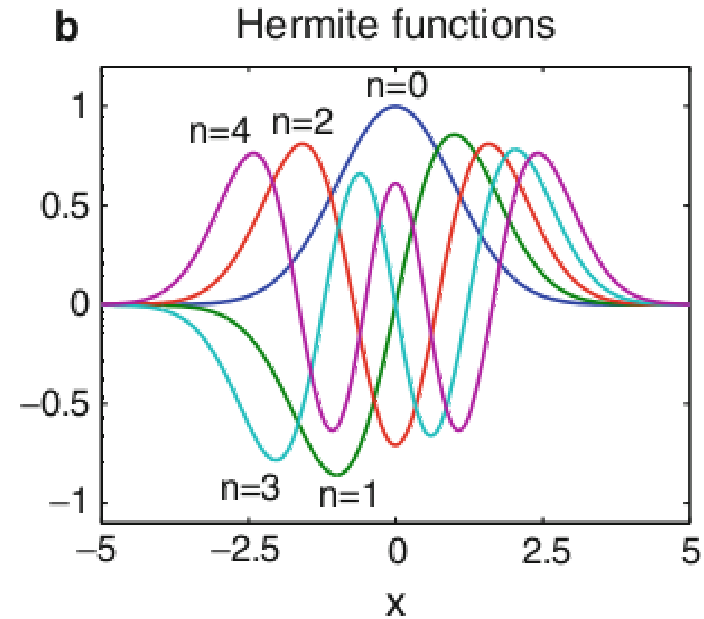
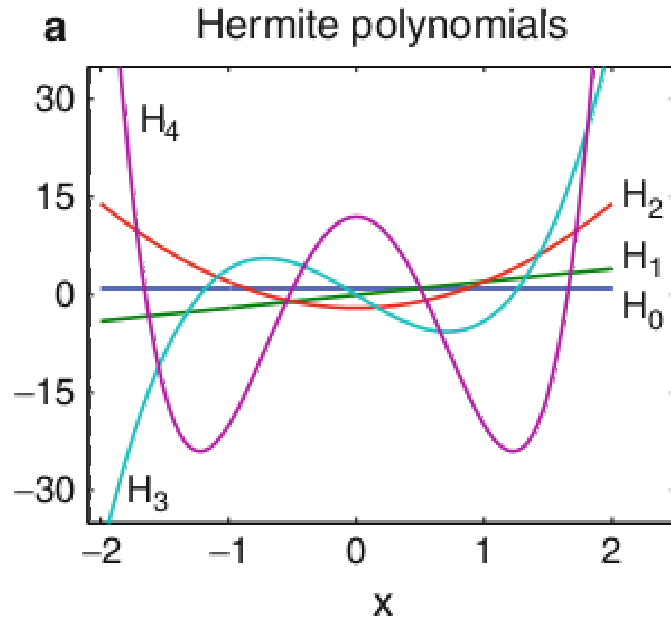
$$H'_n(x) = \lambda_n H_{n-1}(x), \quad n \geq 1. \quad (42)$$

$$H'_n(x) = 2x H_n(x) - H_{n+1}(x), \quad n \geq 0. \quad (43)$$

9. Asymptotics

$$\begin{aligned} \frac{\Gamma(n/2 + 1)}{n!} e^{-x^2/2} H_n(x) &= \cos\left(\sqrt{2n+1}x - \frac{n\pi}{2}\right) \\ &+ \frac{x^3}{6\sqrt{2n+1}} \sin\left(\sqrt{2n+1}x - \frac{n\pi}{2}\right) + O(n^{-1}). \end{aligned} \quad (44)$$

2.2 Hermite functions



$$\hat{H}_n(x) = \frac{1}{\pi^{1/4} \sqrt{2^n n!}} e^{-x^2/2} H_n(x), \quad n \geq 0, \quad x \in \mathbb{R} \quad (45)$$

- Orthogonality

$$\int_{\mathbb{R}} \hat{H}_n(x) \hat{H}_m(x) dx = \delta_{mn}. \quad (46)$$

- Three-term recurrence

$$\begin{aligned}\hat{H}_{n+1}(x) &= x\sqrt{\frac{2}{n+1}}\hat{H}_n(x) - \sqrt{\frac{n}{n+1}}\hat{H}_{n-1}(x), n \geq 1 \\ \hat{H}_0 &= \pi^{-1/4}e^{-x^2/2}, \quad \hat{H}_1(x) = \sqrt{2}\pi^{-1/4}x e^{-x^2/2}.\end{aligned}\tag{47}$$

- Differentiation equation

$$\hat{H}_n''(x) + (2n + 1 - x^2)\hat{H}_n(x) = 0.\tag{48}$$

- Derivatives

$$\begin{aligned}
 \hat{H}'_n(x) &= \sqrt{2n} \hat{H}_{n-1}(x) - x \hat{H}_n(x) \\
 &= \sqrt{\frac{n}{2}} \hat{H}_{n-1}(x) - \sqrt{\frac{n+1}{2}} \hat{H}_{n+1}(x)
 \end{aligned} \tag{49}$$

leads to

$$\int_{\mathbb{R}} \hat{H}'_m(x) \hat{H}'_n(x) \, dx = \begin{cases} -\frac{\sqrt{n(n-1)}}{2}, & m = n-2, \\ n + \frac{1}{2}, & m = n, \\ -\frac{\sqrt{(n+1)(n+2)}}{2}, & m = n+2, \\ 0, & \text{otherwise.} \end{cases} \tag{50}$$

- Asymptotic ($\hat{H}_n(x) \sim n^{-1/4}$, $n \rightarrow \infty$)

$$\hat{H}_n(x) = \pi^{-1/4} \sqrt{2^n n!} \sum_{k=0}^{[n/2]} \frac{(-1)^k}{4^k k! (n-2k)!} (x^{n-2k} e^{-x^2/2}). \quad (51)$$

2.3 Hermite-Gauss Quadrature

Theorem 5. (*Hermite-Gauss Quadrature*) Let $\{x_j\}_{j=0}^N$ be zeros of $H_{N+1}(x)$, and let $\{\omega_j\}_{j=0}^N$ be given by

$$\omega_j = \frac{\sqrt{\pi} 2^N N!}{(N+1) H_N^2(x_j)}, \quad 0 \leq j \leq N. \quad (52)$$

Then,

$$\int_{-\infty}^{+\infty} p(x) e^{-x^2} dx = \sum_{j=0}^N p(x_j) \omega_j, \quad \forall p \in P_{2N+1}. \quad (53)$$

Theorem 6. (*Modified Hermite-Gauss Quadrature*) Let $\{x_j, \omega_j\}_{j=0}^N$ be the Hermite-Gauss quadrature nodes and weights, Define

$$\hat{\omega}_j = e^{x_j^2} \omega_j = \frac{1}{(N+1)\hat{H}_N^2(x_j)}, \quad 0 \leq j \leq N. \quad (54)$$

Then

$$\int_{-\infty}^{+\infty} p(x)q(x) \, dx = \sum_{j=0}^N p(x_j)q(x_j)\hat{\omega}_j, \quad \forall p \cdot q \in \hat{P}_{2N+1}, \quad (55)$$

where

$$\hat{P}_M := \{ \phi: \phi = e^{-x^2/2}\psi, \quad \forall \psi \in P_M \}. \quad (56)$$

Computation of Nodes and Weights

- Zeros $\{x_j\}_{j=0}^N$ of $H_{n+1}(x)$ are eigenvalues of

$$A_{N+1} = \begin{pmatrix} a_0 & \sqrt{b_1} & & & \\ \sqrt{b_1} & a_1 & \sqrt{b_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{b_{N-1}} & a_{N-1} & \sqrt{b_N} \\ & & & \sqrt{b_N} & a_N \end{pmatrix}, \quad (57)$$

$$a_j = 0, \quad 0 \leq j \leq N; \quad b_j = j/2, \quad 1 \leq j \leq N.$$

- Computing $\{\omega_j\}_{j=0}^N$ using (52) is not stable. Instead using

$$\omega_j = e^{-x_j^2} \hat{\omega}_j,$$

$\hat{\omega}_j$ are given by (54).

- Node distribution:

$$\max_j |x_j| \sim \sqrt{2N}, \quad \min_j |x_j - x_{j-1}| \sim 1/\sqrt{N}$$

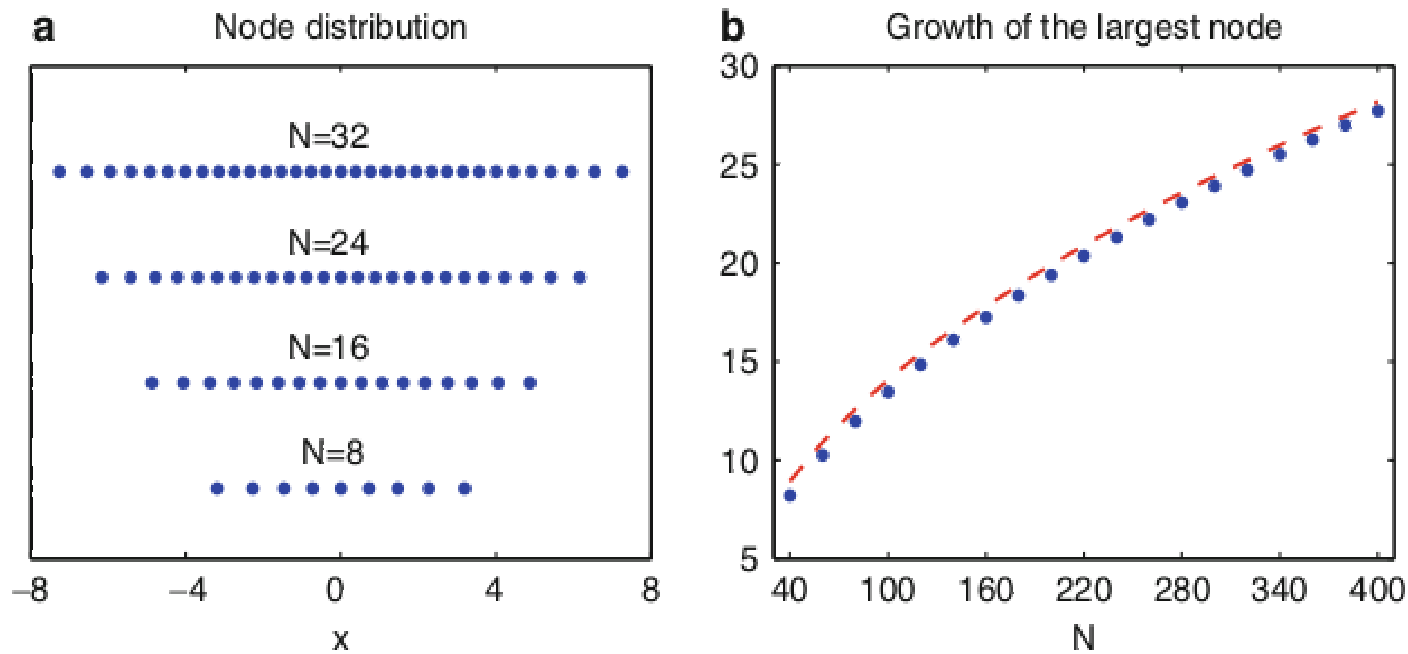


Fig. 7.4 (a) Distribution of the Hermite-Gauss nodes $\{x_j\}_{j=0}^N$ with $N = 8, 16, 24, 32$; (b) Growth of the largest node against N against the asymptotic estimate: $\sqrt{2(N+1)} - (2(N+1))^{1/3}$ (dashed line) with various N

2.4 Interpolation and Discrete Hermite Transforms

- Using Hermite polynomials in P_N :
 $I_N^h v \in P_N$ interpolates $v \in C(\mathbb{R})$ at Hermite-Gauss pts $\{x_j\}_{j=0}^N$:

$$I_N^h v = \sum_{n=0}^N \tilde{v}_n H_n(x); \quad (I_N^h v)(x_j) = v(x_j), \quad 0 \leq j \leq N.$$

Forward discrete transform:

$$\tilde{v}_n = \frac{1}{\gamma_n} \sum_{j=0}^N v(x_j) H_n(x_j) \omega_j, \quad 0 \leq n \leq N \quad (58)$$

Backward discrete transform

$$v(x_j) = \sum_{n=0}^N \tilde{v}_n H_n(x_j), \quad 0 \leq j \leq N. \quad (59)$$

- Using Hermite functions in $\hat{P}_N$
 $\hat{I}_N^h u \in \hat{P}_N$ interpolates $u \in C(\mathbb{R})$ at Hermite-Gauss pts $\{x_j\}_{j=0}^N$:

$$\hat{I}_N^h u = \sum_{n=0}^N \tilde{u}_n \hat{H}_n(x); \quad (\hat{I}_N^h u)(x_j) = u(x_j), \quad 0 \leq j \leq N.$$

Forward discrete transform:

$$\tilde{u}_n = \frac{1}{\gamma_n} \sum_{j=0}^N u(x_j) \hat{H}_n(x_j) \hat{\omega}_j, \quad 0 \leq n \leq N \quad (60)$$

Backward discrete transform

$$u(x_j) = \sum_{n=0}^N \tilde{u}_n \hat{H}_n(x_j), \quad 0 \leq j \leq N. \quad (61)$$

2.5 Differentiation

Differentiation in Physical Space

- Hermite polynomials case (space P_N):

$$\mathbf{u}^{(m)} = D^m \mathbf{u}, \quad m \geq 1, \quad (62)$$

where the entries of D are given by

$$d_{kj} = \begin{cases} \frac{H_N(x_k)}{H_N(x_j)} \frac{1}{x_k - x_j}, & k \neq j, \\ x_k, & k = j. \end{cases} \quad (63)$$

- Hermite functions case (space $\hat{P}_N$):

$$\hat{d}_{kj} = -x_k \delta_{kj} + \frac{e^{-x_k^2/2}}{e^{-x_j^2/2}} d_{kj} = \begin{cases} \frac{\hat{H}_N(x_k)}{\hat{H}_N(x_j)} \frac{1}{x_k - x_j}, & k \neq j, \\ 0, & k = j. \end{cases} \quad (64)$$

Differentiation in Frequency Space

For $u \in P_N$, $u' \in P_{N-1}$:

$$u(x) = \sum_{n=0}^N \hat{u}_n H_n(x), \quad u'(x) = \sum_{n=1}^N \hat{u}_n H'_n(x) = \sum_{n=0}^N \hat{u}_n^{(1)} H_n(x),$$
$$\hat{u}_N^{(1)} = 0; \quad \hat{u}_n^{(1)} = 2(n+1)\hat{u}_{n+1}, \quad n = N-1, N-2, \dots, 0. \quad (65)$$

For $v \in \hat{P}_N$, $v' \in \hat{P}_{N+1}$:

$$v(x) = \sum_{n=0}^N \hat{v}_n \hat{H}_n(x), \quad v'(x) = \sum_{n=0}^N \hat{v}_n \hat{H}'_n(x) = \sum_{n=0}^{N+1} \hat{v}_n^{(1)} \hat{H}_n(x).$$
$$\hat{v}_n^{(1)} = \sqrt{\frac{n+1}{2}} \hat{v}_{n+1} - \sqrt{\frac{n}{2}} \hat{v}_{n-1}, \quad n = N+1, N, \dots, 0. \quad (66)$$

with $\hat{v}_{-1} = \hat{v}_{N+1} = \hat{v}_{N+2} = 0$.

3 Approximation Estimates

3.1 Inverse Inequalities

For Laguerre approximation, $\omega_\alpha = x^\alpha e^{-x}$ and $\hat{\omega}_\alpha = x^\alpha$.

Theorem 7. *For $\alpha > -1$ and any $\phi \in P_N$,*

$$\|\partial_x^m \phi\|_{\omega_{\alpha+m}} \lesssim N^{m/2} \|\phi\|_{\omega_\alpha}, \quad m \geq 0. \quad (67)$$

Corollary 8. *For $\alpha > -1$ and any $\psi \in \hat{P}_N$,*

$$\|\hat{\partial}_x^m \psi\|_{\hat{\omega}_{\alpha+m}} \leq N^{m/2} \|\psi\|_{\hat{\omega}_\alpha}, \quad m \geq 0. \quad (68)$$

Theorem 9. *For $\alpha \geq 0$ and any $\phi \in P_N$,*

$$\|\partial_x^m \phi\|_{\omega_\alpha} \leq N^m \|\phi\|_{\omega_\alpha}, \quad m \geq 0. \quad (69)$$

Corollary 10. *For $\alpha \geq 0$ and any $\psi \in \hat{P}_N$,*

$$\|\hat{\partial}_x^m \psi\|_{\hat{\omega}_\alpha} \lesssim N^m \|\psi\|_{\hat{\omega}_\alpha}, \quad m \geq 0. \quad (70)$$

For the Hermite case, only one weight $\omega(x) = e^{-x^2}$. We have

Theorem 11. *For any $\phi \in P_N$,*

$$\|\partial_x \phi\|_\omega \lesssim N \|\phi\|_\omega,$$

moreover, let $\hat{\partial} = \partial_x + x$. Then for any $\psi \in \hat{P}_N$,

$$\|\hat{\partial}_x \psi\| \lesssim N \|\psi\|.$$

3.2 Orthogonal Projections

Laguerre polynomial $L_{\omega_\alpha}^2$ projection: $\Pi_{N,\alpha}: L_{\omega_\alpha}^2(\mathbb{R}_+) \rightarrow P_N$

$$(\Pi_{N,\alpha}u - u, v_N)_{\omega_\alpha} = 0, \quad \forall v_N \in P_N \quad (71)$$

we have

$$\Pi_{N,\alpha}u = \sum_{n=0}^N \hat{u}_n^{(\alpha)} \mathcal{L}_n^{(\alpha)}(x), \quad \hat{u}_n^{(\alpha)} = \frac{1}{\gamma_n^{(\alpha)}} \left(u, \mathcal{L}_n^{(\alpha)} \right)_{\omega_\alpha}.$$

Define

$$B_\alpha^m(\mathbb{R}_+) := \{u: \partial_x^k u \in L_{\omega_{\alpha+k}}^2(\mathbb{R}_+), \ 0 \leq k \leq m\}, \quad (72)$$

$$\|u\|_{B_\alpha^m} = \left(\sum_{k=0}^m \|\partial_x^k u\|_{\omega_{\alpha+k}}^2 \right)^{1/2}, \quad |u|_{B_\alpha^m} = \|\partial_x^m u\|_{\omega_{\alpha+m}}.$$

Theorem 12. *Let $\alpha > -1$. If $u \in B_\alpha^m(\mathbb{R}_+)$ and $0 \leq m \leq N+1$, then*

$$\|\partial_x^l(\Pi_{N,\alpha}u - u)\|_{\omega_{\alpha+l}} \leq \sqrt{\frac{(N-m+1)!}{(N-l+1)!}} \|\partial_x^m u\|_{\omega_{\alpha+m}}. \quad (73)$$

Laguerre function case: $\hat{\omega}_\alpha = x^\alpha$

For $u \in L^2_{\hat{\omega}_\alpha}(\mathbb{R}_+)$, we have $u e^{x/2} \in L^2_{\omega_\alpha}(\mathbb{R}_+)$. Define

$$\hat{\Pi}_{N,\alpha} u = e^{-x/2} \Pi_{N,\alpha} (u e^{x/2}). \quad \in \hat{P}_N \quad (74)$$

Clearly

$$(\hat{\Pi}_{N,\alpha} u - u, v_N)_{\hat{\omega}_\alpha} = 0, \quad \forall v_N \in \hat{P}_N.$$

Define

$$\hat{B}_\alpha^m(\mathbb{R}_+) := \{u: \hat{\partial}_x^k u \in L^2_{\hat{\omega}_{\alpha+k}}(\mathbb{R}_+), \ 0 \leq k \leq m\}, \quad (75)$$

$$\|u\|_{\hat{B}_\alpha^m} = \left(\sum_{k=0}^m \|\hat{\partial}_x^k u\|_{\hat{\omega}_{\alpha+k}}^2 \right)^{1/2}, \quad |u|_{\hat{B}_\alpha^m} = \|\hat{\partial}_x^m u\|_{\hat{\omega}_{\alpha+m}}.$$

Theorem 13. *Let $\alpha > -1$. If $u \in \hat{B}_\alpha^m(\mathbb{R}_+)$ and $0 \leq m \leq N+1$, then*

$$\|\hat{\partial}_x^l (\Pi_{N,\alpha} u - u)\|_{\hat{\omega}_{\alpha+l}} \leq \sqrt{\frac{(N-m+1)!}{(N-l+1)!}} \|\hat{\partial}_x^m u\|_{\hat{\omega}_{\alpha+m}}. \quad (76)$$

Remark 14. Remarks on Laguerre approximation:

1. The convergence rate is about $N^{(l-m)/2}$, is only half of the classical Jacobi approximation. This is a direct consequence of the linear growth of the eigenvalues in the Sturm–Liouville problem.
2. $B_\alpha^m(\mathbb{R}_+)$ includes functions that do not decay at infinity. A fast convergence rate in $\|\cdot\|_{\omega_{\alpha+l}}$ norm does not mean that the error would decay rapidly for large x .
3. $u \in \hat{B}_\alpha^m(\mathbb{R}_+)$ requires u decays at infinity. So theorem (13) doesn't apply to functions like $\sin(x)$. On the other hand, for $u(x) = (1+x)^{-h}$ and $u(x) = \sin(kx)/(1+x)^h$, we have for both $\|\hat{\partial}_x^m u\|_{\hat{\omega}_{\alpha+m}} < \infty$ if $m < 2h - \alpha - 1$, so we have

$$\|u - \hat{\Pi}_{N,\alpha} u\|_{\hat{\omega}_\alpha} \lesssim N^{-(2h-\alpha-1)/2}. \quad (77)$$

H^1 -type projections. (Here we only consider the case $\alpha = 0$)

Let $\omega(x) = e^{-x}$. Denote

$$H_{0,\omega}^1(\mathbb{R}_+) = \{ u \in H_\omega^1(\mathbb{R}_+) : u(0) = 0 \}, \quad P_N^0 = \{ \phi \in P_N : \phi(0) = 0 \}.$$

Define $\Pi_N^{1,0} : H_{0,\omega}^1(\mathbb{R}_+) \rightarrow P_N^0$ as

$$((u - \Pi_N^{1,0}u)', v'_N)_\omega = 0, \quad \forall v_N \in P_N^0. \quad (78)$$

Theorem 15. *If $u \in H_{0,\omega}^1(\mathbb{R}_+)$ and $\partial_x u \in B_0^{m-1}(\mathbb{R}_+)$, then for $1 \leq m \leq N+1$,*

$$\|\Pi_N^{1,0}u - u\|_{1,\omega} \lesssim \sqrt{\frac{(N-m+1)!}{N!}} \|\partial_x^m u\|_{\omega_{m-1}}, \quad (79)$$

Proof: Let $\phi(x) = \int_0^x \Pi_{N-1,0}u'(y) \, dy$. Then $u - \phi \in H_{0,\omega}^1(\mathbb{R}_+)$.
(B.35b)

$$\|\Pi_N^{1,0}u - u\|_{1,\omega} \leq \|\phi - u\|_{1,\omega} \leq c \|\partial_x(\phi - u)\|_\omega$$

Laguerre function case

For $u \in H_0^1(\mathbb{R}_+)$, we have $u e^{x/2} \in H_{0,\omega}^1(\mathbb{R}_+)$. Define

$$\hat{\Pi}_N^{1,0} u = e^{-x/2} \Pi_N^{1,0}(u e^{x/2}) \in \hat{P}_N^0.$$

Theorem 16. *For any $u \in H_0^1(\mathbb{R}_+)$, we have*

$$\left((u - \hat{\Pi}_N^{1,0} u)', v_N' \right) + \frac{1}{4} (u - \hat{\Pi}_N^{1,0} u, v_N) = 0, \quad \forall v_N \in \hat{P}_N^0. \quad (80)$$

Let $\hat{\partial}_x = \partial_x + \frac{1}{2}$. If $u \in H_0^1(\mathbb{R}_+)$ and $\hat{\partial}_x u \in \hat{B}_n^{m-1}(\mathbb{R}_+)$, then

$$\|\hat{\Pi}_N^{1,0} u - u\|_1 \leq c \sqrt{\frac{(N - m + 1)!}{N!}} \|\hat{\partial}_x^m u\|_{\hat{\omega}_{m-1}}, \quad (81)$$

where c is a positive constant independent of m, N and u .

H^2 -type orthogonal projections

Define

$$H_{0,\omega}^2(\mathbb{R}_+) = \{ v \in H_\omega^2(\mathbb{R}_+) : v(0) = v'(0) = 0 \}, \quad X_N = H_{0,\omega}^2(\mathbb{R}_+) \cap P_N,$$

$$H_0^2(\mathbb{R}_+) = \{ v \in H^2(\mathbb{R}_+) : v(0) = v'(0) = 0 \}, \quad \hat{X}_N = H_0^2(\mathbb{R}_+) \cap \hat{P}_N.$$

Define $\Pi_N^{2,0} : H_{0,\omega}^2(\mathbb{R}_+) \rightarrow X_N$, as

$$\left((v - \Pi_N^{2,0} u)'' , v_N'' \right)_\omega = 0, \quad \forall v_N \in X_N. \quad (82)$$

Define $\hat{\Pi}_N^{2,0} : H_0^2(\mathbb{R}_+) \rightarrow \hat{X}_N$ as

$$\hat{\Pi}_N^{2,0} u = e^{-x/2} \Pi_N^{2,0} (u e^{x/2}). \quad (83)$$

Theorem 17. *If $v \in H_{0,\omega}^2(\mathbb{R}_+)$ and $\partial_x^2 v \in B_0^{m-2}(\mathbb{R}_+)$ with $2 \leq m \leq N+1$, then we have*

$$\|\Pi_N^{2,0}v - v\|_{2,\omega} \leq c \sqrt{\frac{(N-m+1)!}{(N-1)!}} \|\partial_x^m v\|_{\omega_{m-2}}. \quad (84)$$

For $u \in H_0^2(\mathbb{R}_+)$ and all $u_N \in \hat{X}_N$, we have

$$((u - \hat{\Pi}_N^{2,0}u)'', u_N'') + \frac{1}{2}((u - \hat{\Pi}_N^{2,0}u)', u_N') + \frac{1}{16}(u - \hat{\Pi}_N^{2,0}u, u_N) = 0. \quad (85)$$

Moreover, if $u \in H_0^2(\mathbb{R}_+)$ and $\hat{\partial}_x^2 u \in \hat{B}_0^{m-2}(\mathbb{R}_+)$ with $2 \leq m \leq N+1$, then

$$\|\hat{\Pi}_N^{2,0}u - u\|_{2,\hat{\omega}} \leq c \sqrt{\frac{(N-m+1)!}{(N-1)!}} \|\hat{\partial}_x^m u\|_{\hat{\omega}_{m-2}}. \quad (86)$$

Hermite projections ($\omega(x) = e^{-x^2}$)

$\Pi_N: L_\omega^2(\mathbb{R}) \rightarrow P_N$:

$$(u - \Pi_N u, v_N)_\omega = 0, \quad \forall v_N \in P_N. \quad (87)$$

Clearly

$$\Pi_N u(x) = \sum_{n=0}^N \hat{u}_n H_n(x), \quad \hat{u}_n = \frac{1}{\gamma_n} (u, H_n)_\omega.$$

Theorem 18. *For any $u \in H_\omega^m(\mathbb{R})$ with $0 \leq m \leq N+1$,*

$$\|\partial_x^l(\Pi_N u - u)\|_\omega \leq 2^{(l-m)/2} \sqrt{\frac{(N-m+1)!}{(N-l+1)!}} \|\partial_x^m\|_\omega, \quad 0 \leq l \leq m. \quad (88)$$

Reamrks: The $L_\omega^2(\mathbb{R})$ -orthogonal projection is simultaneously optimal in the $H_\omega^l(\mathbb{R})$ -norm with $l \geq 1$.

Hermite function approximation

For $u \in L^2(\mathbb{R})$, we have $u e^{x^2/2} \in L^2_\omega(\mathbb{R})$, define

$$\hat{\Pi}_N u := e^{-x^2/2} \Pi_N(u e^{x^2/2}) \in \hat{P}_N, \quad (89)$$

which satisfies

$$(u - \hat{\Pi}_N u, v_N) = (u e^{x^2/2} - \Pi_N(u e^{x^2/2}), v_N e^{x^2/2})_\omega = 0, \forall v_N \in \hat{P}_N.$$

Theorem 19. *Let $\hat{\partial}_x = \partial_x + x$. For $\hat{\partial}_x^m u \in L^2(\mathbb{R})$ with $0 \leq m \leq N+1$,*

$$\|\hat{\partial}_x^l(\hat{\Pi}_N u - u)\| \lesssim 2^{(l-m)/2} \sqrt{\frac{(N-m+1)!}{(N-l+1)!}} \|\hat{\partial}_x^m u\|, \quad 0 \leq l \leq m. \quad (90)$$

Theorem 20. *For any $\hat{\partial}_x^m u \in L^2(\mathbb{R})$ with $2 \leq m \leq N+1$,*

$$\|\partial_x^l(\hat{\Pi}_N u - u)\| \lesssim \sqrt{\frac{(N-m+1)!}{2^m(N-l+1)!}} \|\hat{\partial}_x^m u\|, \quad l = 0, 1, 2. \quad (91)$$

3.3 Interpolations

Theorem 21. (Laguerre-Gauss interpolation[Guo et al 2006b])

Let $\alpha > -1$. If $u \in C(\mathbb{R}_+) \cap B_\alpha^m(\mathbb{R}_+)$ and $\partial_x u \in B_\alpha^{m-1}(\mathbb{R}_+)$ with $1 \leq m \leq N+1$, then

$$\left\| I_N^{(\alpha)} u - u \right\|_{\omega_\alpha} \lesssim \sqrt{\frac{(N-m+1)!}{N!}} \left(\|\partial_x^m u\|_{\omega_{\alpha+m-1}} + \sqrt{\ln N} \|\partial_x^m u\|_{\omega_{\alpha+m}} \right).$$

Theorem 22. Let $\alpha > -1$. If $u \in C(\mathbb{R}_+) \cap \hat{B}_\alpha^m(\mathbb{R}_+)$ and $\hat{\partial}_x u \in \hat{B}_\alpha^{m-1}(\mathbb{R}_+)$ with $1 \leq m \leq N+1$ then

$$\left\| \hat{I}_N^{(\alpha)} u - u \right\|_{\hat{\omega}_\alpha} \lesssim \sqrt{\frac{(N-m+1)!}{N!}} \left(\|\hat{\partial}_x^m u\|_{\hat{\omega}_{\alpha+m-1}} + \sqrt{\ln N} \|\hat{\partial}_x^m u\|_{\hat{\omega}_{\alpha+m}} \right)$$

Hermite Interpolation

Theorem 23. ([Guo and Xu 2000]) For $u \in C(\mathbb{R}) \cap H_\omega^m(\mathbb{R})$ with $m \geq 1$, we have

$$\|\partial_x^l(I_N^h u - u)\|_\omega \lesssim N^{\frac{1}{6} + \frac{l-m}{2}} \|\partial_x^m u\|_\omega, \quad 0 \leq l \leq m. \quad (92)$$

Theorem 24. Let $\hat{\partial}_x = \partial_x + x$. For $u \in C(\mathbb{R})$ and $\hat{\partial}_x^m u \in L^2(\mathbb{R})$ with fixed $m \geq 1$, we have

$$\|\hat{\partial}_x^l(\hat{I}_N^h u - u)\| \lesssim N^{\frac{1}{6} + \frac{l-m}{2}} \|\hat{\partial}_x^m u\|, \quad 0 \leq l \leq m. \quad (93)$$

4 Spectral Methods Using Laguerre and Hermite Functions

4.1 Laguerre-Galerkin Method

$$\begin{aligned} -u_{xx} + \gamma u &= f, \quad x \in \mathbb{R}_+, \gamma > 0; \\ u(0) &= 0, \quad \lim_{x \rightarrow +\infty} u(x) = 0. \end{aligned} \tag{94}$$

Weak formulation (for $f \in (H_0^1(\mathbb{R}_+))'$)

$$\begin{cases} \text{Find } u \in H_0^1(\mathbb{R}_+) \text{ such that} \\ a(u, v) := (u', v') + \gamma(u, v) = (f, v), \quad \forall v \in H_0^1(\mathbb{R}_+) \end{cases} \tag{95}$$

Laguerre spectral-Galerkin approximation to (94)

$$\begin{cases} \text{Find } u_N \in \hat{P}_N^0 \text{ such that} \\ a(u_N, v_N) = (\hat{I}_N f, v_N), \quad \forall v_N \in \hat{P}_N^0 \end{cases} \tag{96}$$

Define

$$\hat{\phi}_k(x) = (\mathcal{L}_k(x) - \mathcal{L}_{k+1}(x)) e^{-x/2} = \hat{\mathcal{L}}_k(x) - \hat{\mathcal{L}}_{k+1}(x) \quad (97)$$

then $\hat{P}_N^0 = \text{span}\{ \hat{\phi}_0, \hat{\phi}_1, \dots, \hat{\phi}_{N-1} \}$. By setting

$$\begin{aligned} u_N &= \sum_{k=0}^{N-1} \hat{u}_k \hat{\phi}_k, & \mathbf{u} &= (\hat{u}_0, \hat{u}_1, \dots, \hat{u}_{N-1})^T; \\ f_j &= (\hat{I}_N f, \hat{\phi}_j), & \mathbf{f} &= (f_0, f_1, \dots, f_{N-1})^T; \\ s_{jk} &= (\hat{\phi}'_k, \hat{\phi}'_j), & \mathbf{S} &= (s_{jk})_{0 \leq j, k \leq N-1}; \\ m_{jk} &= (\hat{\phi}_k, \hat{\phi}_j), & \mathbf{M} &= (m_{jk})_{0 \leq j, k \leq N-1} \end{aligned}$$

we find $\mathbf{M}$ is a symmetric tridiagonal matrix and $\mathbf{S} = \mathbf{I} - \frac{1}{4}\mathbf{M}$, so (96) reduces to

$$(\mathbf{I} + (\gamma - \frac{1}{4})\mathbf{M})\mathbf{u} = \mathbf{f}. \quad (98)$$

Theorem 25. *If $u \in H_0^1(\mathbb{R}_+)$, $\hat{\partial}_x u \in \hat{B}_0^{m-1}(\mathbb{R}_+)$, $f \in C(\bar{\mathbb{R}}_+) \cap \hat{B}_0^k(\mathbb{R}_+)$ and $\hat{\partial}_x f \in \hat{B}_0^{k-1}(\mathbb{R}_+)$ with $1 \leq k, m \leq N+1$, then we have*

$$\begin{aligned} \|u - u_N\|_1 &\lesssim \sqrt{\frac{(N-m+1)!}{N!}} \|\hat{\partial}_x^m u\|_{\hat{\omega}_{m-1}} \\ &\quad + \sqrt{\frac{(N-k+1)!}{N!}} \left(\|\hat{\partial}_x^k f\|_{\hat{\omega}_{k-1}} + \sqrt{\ln N} \|\hat{\partial}_x^k f\|_{\hat{\omega}_k} \right). \end{aligned} \quad (99)$$

Proof. Let $e_N = u_N - \hat{\Pi}_N^{1,0} u$ and $\tilde{e}_N = u - \hat{\Pi}_N^{1,0} u$, then by

$$a(u_N - u, v_N) = (\hat{I}_N f - f, v_N), \quad \forall v_N \in \hat{P}_N^0$$

$$a(e_N, v_N) = a(\tilde{e}_N, v_N) + (\hat{I}_N f - f, v_N), \quad \forall v_N \in \hat{P}_N^0.$$

Taking $v_N = e_N$, we find

$$\|e_N\|_1 \leq c(\|\tilde{e}_N\|_1 + \|\hat{I}_N f - f\|).$$

□

4.2 Hermite–Galerkin Method

$$-u_{xx} + \gamma u = f, \quad x \in \mathbb{R}, \quad \gamma > 0; \quad \lim_{|x| \rightarrow \infty} u(x) = 0. \quad (100)$$

Weak formulation

$$\begin{cases} \text{Find } u \in H^1(\mathbb{R}) \text{ such that} \\ (\partial_x u, \partial_x v) + \gamma(u, v) = (f, v), \quad \forall v \in H^1(\mathbb{R}). \end{cases} \quad (101)$$

Hermite–Galerkin method

$$\begin{cases} \text{Find } u_N \in \hat{P}_N \text{ such that} \\ (\partial_x u, \partial_x v) + \gamma(u, v) = (\hat{I}_N^h f, v_N), \quad \forall v_N \in \hat{P}_N. \end{cases} \quad (102)$$

Theorem 26. *Let $\gamma > 0$ and $\hat{\partial}_x = \partial_x + x$. If $u \in H^1(\mathbb{R})$ with $\hat{\partial}_x^m u \in L^2(\mathbb{R})$, and $f \in C(\mathbb{R})$ with $\hat{\partial}_x^k f \in L^2(\mathbb{R})$ and fixed $k, m \geq 1$, then*

$$\|u_N - u\|_1 \lesssim N^{\frac{1-m}{2}} \|\hat{\partial}_x^m u\| + N^{\frac{1}{6} - \frac{k}{2}} \|\hat{\partial}_x^k f\|. \quad (103)$$

4.3 Numerical Results

Exact solution $u(x)$	$x \in (0, \infty)$	$x \in (-\infty, \infty)$
$u_1(x)$	$e^{-x} \sin(kx)$	$e^{-x^2} \sin(kx)$
$u_2(x)$	$\frac{1}{(1+x)^h}$	$\frac{1}{(1+x^2)^h}$
$u_3(x)$	$\frac{\sin(kx)}{(1+x)^h}$	$\frac{\sin(kx)}{(1+x^2)^h}$

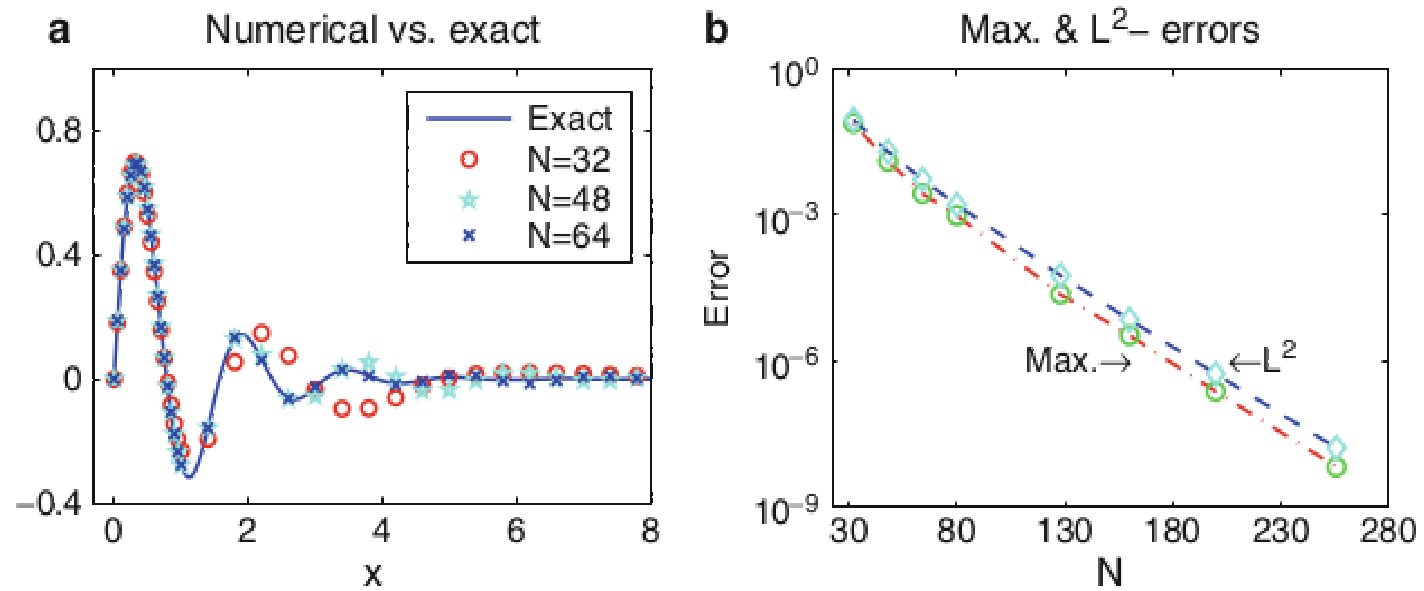


Figure 1. (Laguerre) Exponential decay solution $u_1(x)$ with $k=4$, $\gamma=1$.

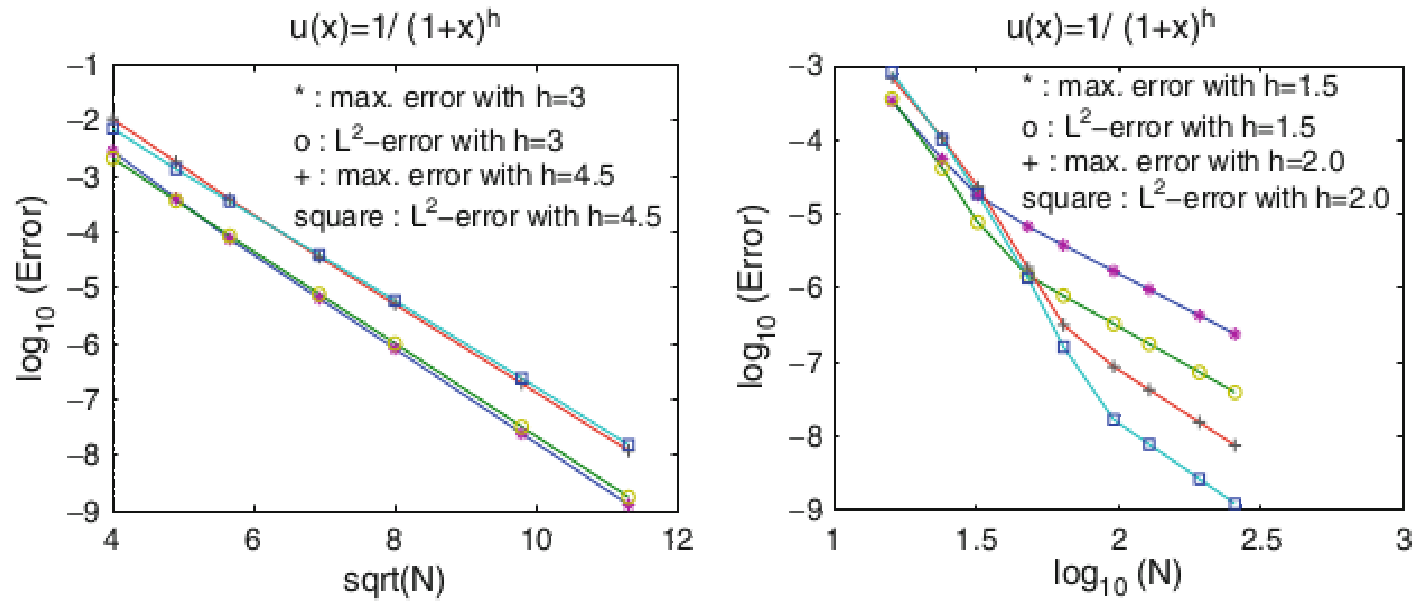


Figure 2. (Laguerre) Algebraic decay solution $u_2(x)$: different h and N .

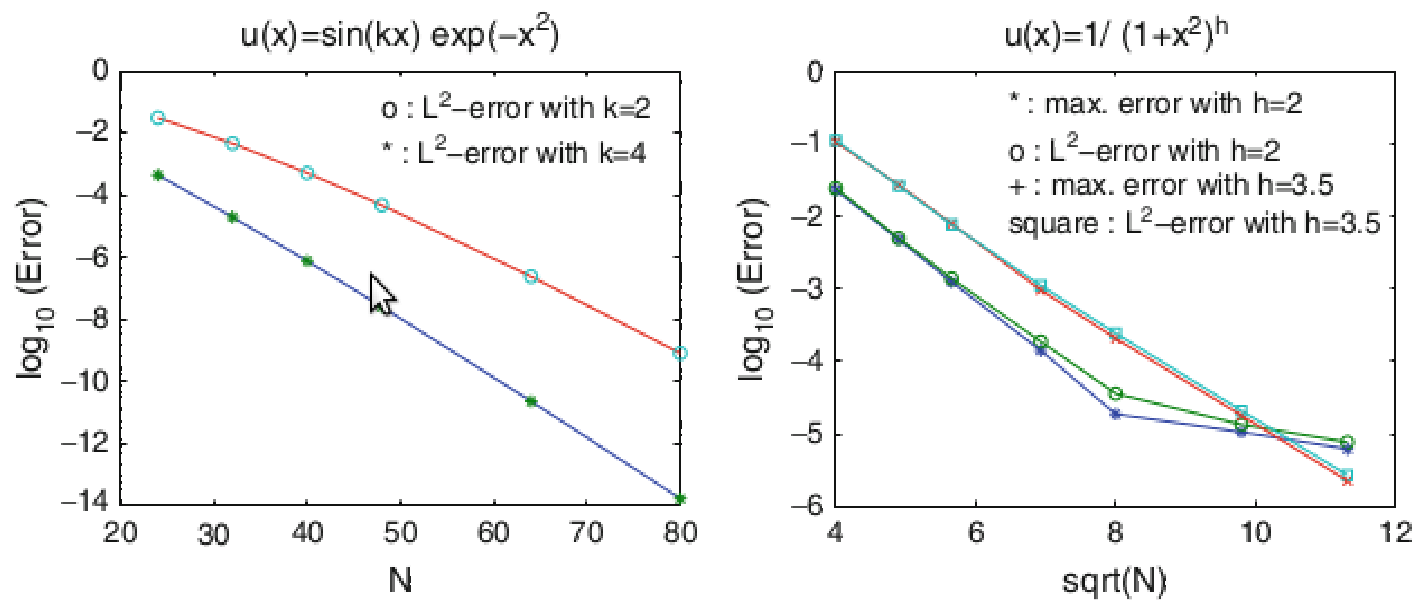


Figure 3. (Hermite) Exponential decay $u_1(x)$, Algebraic decay $u_2(x)$.

4.4 Scaling Factor

Assume that

$$|u(x)| \leq \varepsilon \quad \text{for } x > M.$$

Scaling factor (x_N is the largest L-G-R point)

$$\beta_N = x_N / M,$$

Scaled equation

$$-\beta_N^2 v_{yy} + \gamma v = g(y); \quad v(0) = 0, \quad \lim_{y \rightarrow +\infty} v(y) = 0. \quad (104)$$

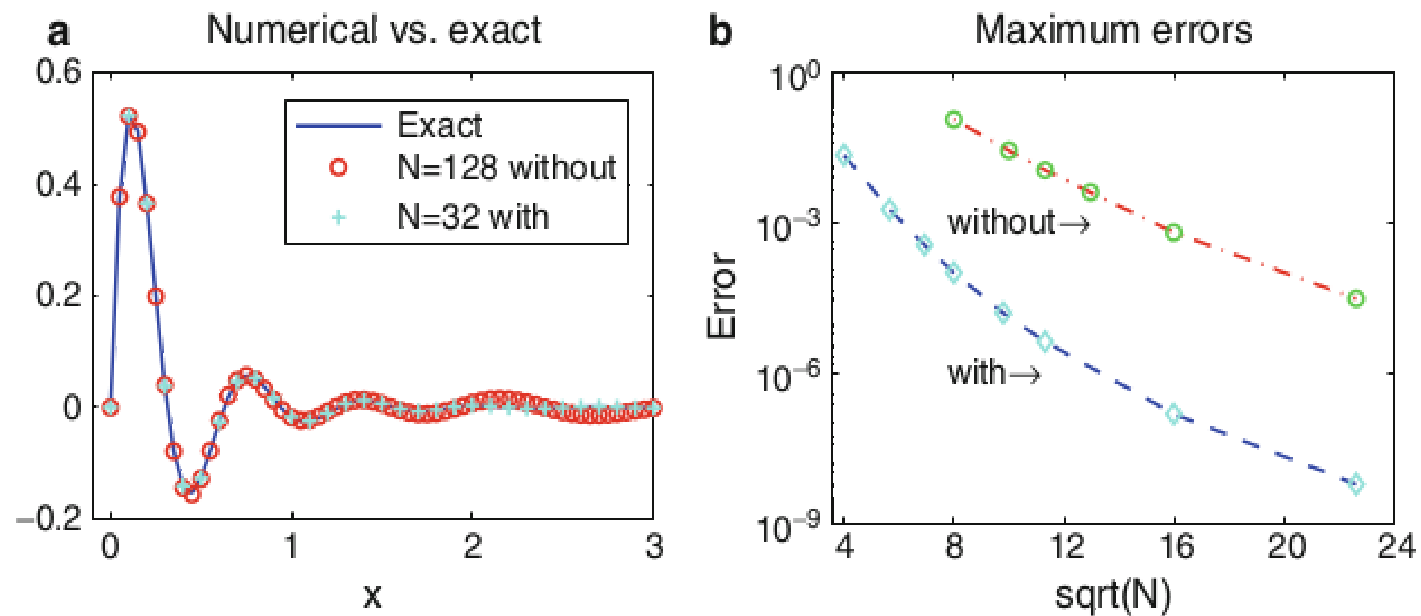


Figure 4. Scaling effects. $\beta_N = 15$.

5 Mapped Spectral Methods

5.1 Mappings

$$x = g(y; s), \quad y \in (-1, 1), \quad x \in \Lambda := (0, +\infty) \text{ or } (-\infty, +\infty) \quad (105)$$

with $s > 0$ and

$$\begin{aligned} \frac{dx}{dy} &= g'(y; s) > 0. \\ g(-1; s) &= 0, \quad g(1; s) = +\infty, & \text{if } \Lambda = (0, +\infty) \\ g(\pm 1; s) &= \pm\infty, & \text{if } \Lambda = (-\infty, +\infty) \end{aligned} \quad (106)$$

1. Mapping between $x \in (-\infty, +\infty)$ and $y \in (-1, 1)$ with $s > 0$.

- Algebraic mapping:

$$x = \frac{s y}{\sqrt{1 - y^2}}, \quad y = \frac{x}{\sqrt{x^2 + s^2}}. \quad (107)$$

- Logarithmic mapping:

$$x = \frac{s}{2} \ln \frac{1 + y}{1 - y}, \quad y = \tanh \frac{x}{s} \quad (108)$$

- Exponential mapping:

$$x = \sinh(s y), \quad y = \frac{1}{s} \ln(x + \sqrt{x^2 + 1}), \quad (109)$$

where $y \in (-1, 1)$, $x \in (-L_s, L_s)$, and $L_s = \sinh(s)$.

2. Mapping between $x \in (0, +\infty)$ and $y \in (-1, 1)$ with $s > 0$:

- Algebraic mapping:

$$x = s \frac{1+y}{1-y}, \quad y = \frac{x-s}{x+s}. \quad (110)$$

- Logarithmic mapping

$$x = \frac{s}{2} \ln \frac{3+y}{1-y}, \quad y = 1 - 2 \tanh \left(\frac{x}{s} \right). \quad (111)$$

- Exponential mapping

$$x = \sinh \left(s \frac{1+y}{2} \right), \quad y = \frac{2}{s} \ln(x + \sqrt{x^2 + 1}) - 1, \quad (112)$$

where $x \in (0, L_s)$, $L_s = \sinh(s)$.

5.2 Approximation by Mapped Jacobi Polynomials

For the algebraic mapping, we define rational Jacobi polynomials:

$$j_{n,s}^{\alpha,\beta}(x) := J_n^{\alpha,\beta}(y) \quad (113)$$

then

$$\int_{\Lambda} j_{n,s}^{\alpha,\beta}(x) j_{m,s}^{\alpha,\beta}(x) \omega_s^{\alpha,\beta}(x) dx = \gamma_n^{\alpha,\beta} \delta_{mn}, \quad (114)$$

where $\gamma_n^{\alpha,\beta} = (J_n^{\alpha,\beta}, J_n^{\alpha,\beta})_{\omega^{\alpha,\beta}}$ and

$$\omega_s^{\alpha,\beta}(x) = \omega^{\alpha,\beta}(y) \frac{dy}{dx} = \omega^{\alpha,\beta}(y) \left(\frac{dx}{dy} \right)^{-1} > 0 \quad (115)$$

Note that for mapping (107) and (110), we have respectively

$$\frac{dx}{dy} = \frac{s}{\sqrt{1-y^2}^3} = s \omega^{-\frac{3}{2}, -\frac{3}{2}}, \quad \frac{dx}{dy} = \frac{2s}{(1-y)^2} = 2s \omega^{-2,0}.$$

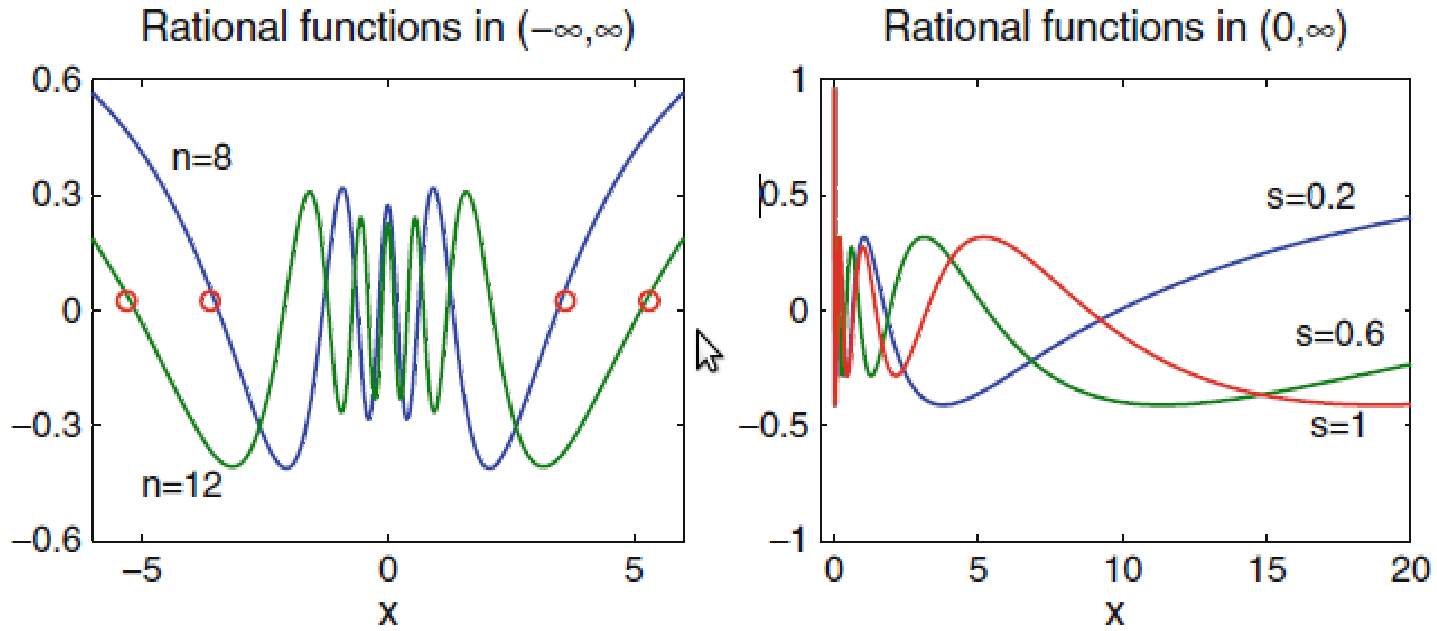


Figure 5. (Left) Graph of $j_{n,1}^{0,0}(x)$ with $n = 8, 12$ using mapping (107). (Right) Graphs of $j_{8,s}^{0,0}(x)$ with $s = 0.2, 0.6, 1$ using mapping (110).

Approximation

$$V_{N,s}^{\alpha,\beta} = \text{span}\{j_{n,s}^{\alpha,\beta}(x) : n = 0, 1, \dots, N\}, \quad s > 0. \quad (116)$$

Consider the orthogonal projection $\pi_{N,s}^{\alpha,\beta} : L_{\omega_s^{\alpha,\beta}}^2(\Lambda) \rightarrow V_{N,s}^{\alpha,\beta}$:

$$(\pi_{N,s}^{\alpha,\beta} u - u, v_N)_{\omega_s^{\alpha,\beta}} = 0, \quad \forall v_N \in V_{N,s}^{\alpha,\beta}. \quad (117)$$

For a given mapping $x = g(y, s)$, define

$$a_s(x) := \frac{dx}{dy} (> 0), \quad U_s(y) := u(x) = u(g(y, s)). \quad (118)$$

Then by defining $D_x u := a_s \frac{du}{dx}$, we have

$$\frac{dU_s}{dy} = a_s \frac{du}{dx} = D_x u, \quad \frac{d^k U_s}{dy^k} = D_x^k u. \quad (119)$$

Define space

$$\tilde{B}_{\alpha,\beta}^m(\Lambda) = \left\{ u: u \text{ is measurable in } \Lambda \text{ and } \|u\|_{\tilde{B}_{\alpha,\beta}^m} < \infty \right\} \quad (120)$$

equipped with the norm and semi-norm

$$\|u\|_{\tilde{B}_{\alpha,\beta}^m} = \left(\sum_{k=0}^m \|D_x^k u\|_{\omega_s^{\alpha+k,\beta+k}}^2 \right)^{1/2}, \quad |u|_{\tilde{B}_{\alpha,\beta}^m} = \|D_x^m u\|_{\omega_s^{\alpha+m,\beta+m}}.$$

Theorem 27. *Let $\alpha, \beta > -1$. If $u \in \tilde{B}_{\alpha,\beta}^m(\Lambda)$, then for $0 \leq m \leq N+1$,*

$$\left\| \pi_{N,s}^{\alpha,\beta} u - u \right\|_{\omega_s^{\alpha,\beta}} \lesssim \sqrt{\frac{(N-m+1)!}{(N+1)!}} (N+m)^{-\frac{m}{2}} \|D_x^m u\|_{\omega_s^{\alpha+m,\beta+m}}, \quad (121)$$

and for $1 \leq m \leq N+1$,

$$\left\| \partial_x \left(\pi_{N,s}^{\alpha,\beta} u - u \right) \right\|_{\tilde{\omega}_s^{\alpha,\beta}} \lesssim \sqrt{\frac{(N-m+1)!}{N!}} (N+m)^{(1-m)/2} \|D_x^m u\|_{\omega_s^{\alpha+m,\beta+m}}, \quad (122)$$

where $\tilde{\omega}_s^{\alpha,\beta}(x) = \omega^{\alpha+1,\beta+1} g'(y; s)$, $y = h(x; s)$.

For algebraic mapping on $(0, +\infty)$

1. For $u(x) = \frac{1}{(1+x)^h}$, $\|D_x^m u\|_{\omega_s^{\alpha+m, \beta+m}} < \infty$ if $m < 2h + \alpha + 1$:

$$\|u - \pi_{N,s}^{\alpha, \beta} u\|_{\omega_s^{\alpha, \beta}} \lesssim N^{-(2h+\alpha+1)}, \quad (u(x) = (1+x)^{-h}) \quad (123)$$

2. For $u(x) = \frac{\sin(kx)}{(1+x)^h}$, $\|D_x^m u\|_{\omega_s^{\alpha+m, \beta+m}} < \infty$ if $m < \frac{2h + \alpha + 1}{3}$:

$$\|u - \pi_{N,s}^{\alpha, \beta} u\|_{\omega_s^{\alpha, \beta}} \lesssim N^{-(2h+\alpha+1)/3}, \quad \left(u(x) = \frac{\sin(kx)}{(1+x)^h}\right) \quad (124)$$

For algebraic mapping on $(-\infty, +\infty)$

1. Algebraic decay

$$\|u - \pi_{N,s}^{\alpha, \beta} u\|_{\omega_s^{\alpha, \beta}} \lesssim N^{-(2h+\alpha+1)}, \quad (u(x) = (1+x^2)^{-h}) \quad (125)$$

2. Algebraic decay with oscillation

$$\|u - \pi_{N,s}^{\alpha, \beta} u\|_{\omega_s^{\alpha, \beta}} \lesssim N^{-(2h+\alpha+1)/2}, \quad (u(x) = \frac{\sin(kx)}{(1+x^2)^h}) \quad (126)$$

Remark 28.

1. For $u = (1 + x)^{-h}$ and $u = (1 + x^2)^{-h}$
 - a. if h positive integer, expressed exactly by finite sum of mapped rational functions
 - b. for other case, algebraic convergence rate but faster than approx. by Laguerre functions or Hermite functions.
2. For solutions with oscillation $u(x) = \frac{\sin(kx)}{(1+x)^h}, \frac{\sin(kx)}{(1+x^2)^h}$. The convergence rates are much slower than solution without oscillations. And also slower than Laguerre functions and Hermite functions methods.
3. For solutions with exponential decay at infinity, the convergence rate is faster than any algebraic rate. $\sim e^{-c\sqrt{N}}$.

Mapped Interpolation

Given Jacobi-Gauss points $\{\xi_{N,j}^{\alpha,\beta}\}_{j=0}^N$, define $\zeta_{N,j,s}^{\alpha,\beta} := g(\xi_{N,j}^{\alpha,\beta}; s)$, and mapped Jacobi-Gauss interpolation $I_{N,s}^{\alpha,\beta}: C(\Lambda) \rightarrow V_{N,s}^{\alpha,\beta}$ as:

$$I_{N,s}^{\alpha,\beta} u \in V_{N,s}^{\alpha,\beta} \text{ s.t. } (I_{N,s}^{\alpha,\beta} u)(\zeta_{N,j,s}^{\alpha,\beta}) = u(\xi_{N,j}^{\alpha,\beta}), j = 0, 1, \dots, N. \quad (127)$$

Theorem 29. *Let $\alpha, \beta > -1$. If $u \in \tilde{B}_{\alpha,\beta}^m(\Lambda)$ with $1 \leq m \leq N+1$, then*

$$\begin{aligned} & \|\partial_x(I_{N,s}^{\alpha,\beta} u - u)\|_{\tilde{\omega}_s^{\alpha,\beta} + N} \|I_{N,s}^{\alpha,\beta} u - u\|_{\omega_s^{\alpha,\beta}} \\ & \lesssim \sqrt{\frac{(N-m+1)!}{N!}} (N+m)^{(1-m)/2} \|D_x^m u\|_{\omega_s^{\alpha+m,\beta+m}}. \end{aligned} \quad (128)$$

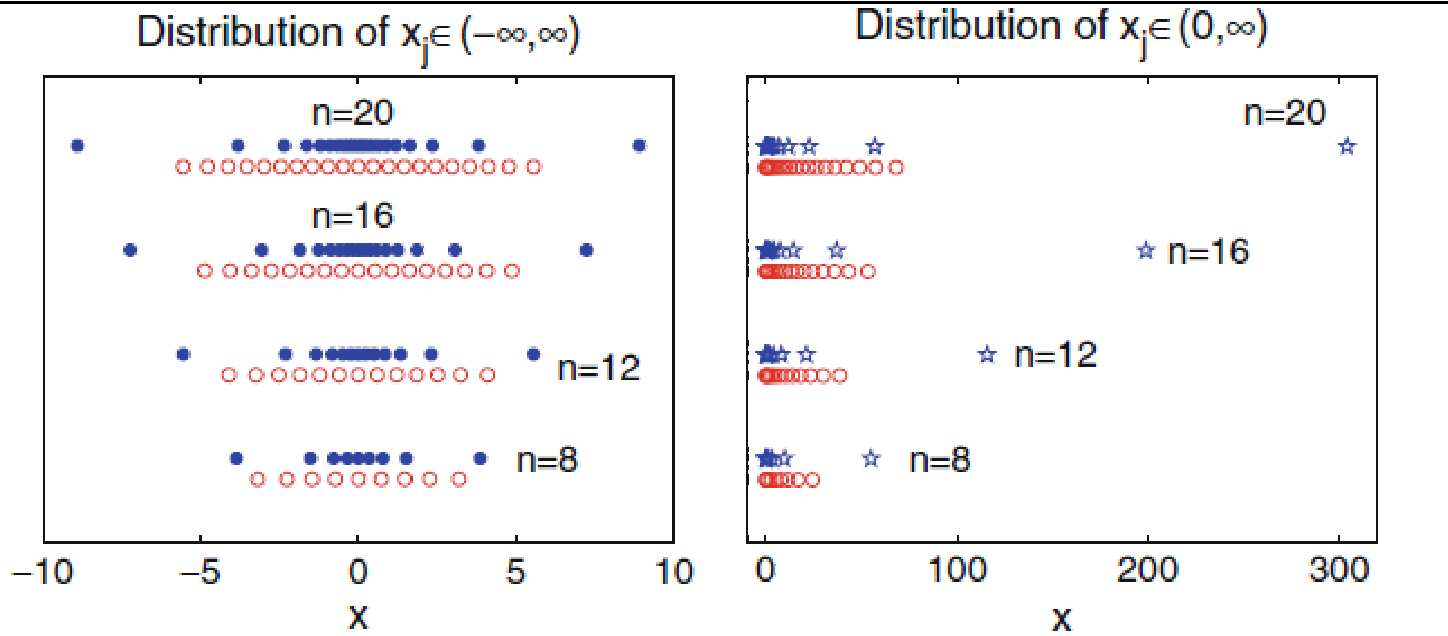


Figure 6. (Left): Hermite–Gauss points (“o”) vs. mapped Legendre–Gauss points using the algebraic map (107) with $s = 1$ (“•”).

$\min_j |x_{j+1} - x_j| \sim O(N^{-1})$ for mapped Legendre–Gauss points.

(Right) Laguerre–Gauss–Radau points (“o”) vs. mapped Legendre–Gauss–Radau points using the algebraic map (110) with $s = 1$ (“★”).

$\min_j |x_{j+1} - x_j| \sim O(N^{-2})$ for mapped Legendre–Gauss–Radau points.

5.3 Spectral Methods Using Mapped Jacobi Polynomials

$$\gamma u - \partial_x(a(x)\partial_x u) = f, \quad x \in \Lambda = (-\infty, +\infty), \quad \gamma > 0 \quad (129)$$

For a given map $x = g(y; s)$, the weighted weak form

$$\begin{cases} \text{Find } u \in \tilde{B}_{\alpha, \beta}^1(\Lambda) \text{ such that} \\ \gamma(u, v)_{\omega_s^{\alpha, \beta}} + (a(x)\partial_x u, \partial_x(v \omega_s^{\alpha, \beta})) = (f, v)_{\omega_s^{\alpha, \beta}}, \forall v \in \tilde{B}_{\alpha, \beta}^1(\Lambda). \end{cases} \quad (130)$$

The corresponding mapped Jacobi–Galerkin method is

$$\begin{cases} \text{Find } u_N \in V_{N, s}^{\alpha, \beta} \text{ such that } \forall v_N \in V_{N, s}^{\alpha, \beta} \\ \gamma(u_N, v_N)_{\omega_s^{\alpha, \beta}} + (a(x)\partial_x u_N, \partial_x(v_N \omega_s^{\alpha, \beta})) = (I_{N, s}^{\alpha, \beta} f, v_N)_{\omega_s^{\alpha, \beta}}. \end{cases} \quad (131)$$

A second approach: Jacobi approximation for transformed problem:

$$\gamma U_s(y) - \frac{1}{g'(y; s)} \partial_y \left(\frac{a(g(y; s))}{g'(y; s)} \partial_y U_s(y) \right) = F_s(y), \quad (132)$$

where $U_s(y) = u(g(y; s))$ and $F_s(y) = f(g(y; s))$.

Let $\hat{\omega}_s^{\alpha, \beta}(y) = \omega^{\alpha, \beta}(y) g'(y; s)$. Jacobi-Galerkin method for (132) is

$$\begin{cases} \text{Find } \tilde{u}_N \in P_N \text{ s.t. } \forall \tilde{v}_N \in P_N \\ \gamma(\tilde{u}_N, \tilde{v}_N)_{\omega^{\alpha, \beta}} + \left(\frac{a(g(y; s))}{g'(y; s)} \partial_y \tilde{u}_N, \partial_y (\tilde{v}_N \hat{\omega}_s^{\alpha, \beta}) \right) = (I_N^{\alpha, \beta} F_s, \tilde{v}_N)_{\omega^{\alpha, \beta}} \end{cases} \quad (133)$$

This approach is in general more difficult to analyze, but can be easily implemented using the standard Jacobi–collocation method.

Error Estimates for a Model Problem

$$\gamma u(x) - \partial_x^2 u(x) = f(x), \quad x \in \Lambda = (0, \infty), \quad \gamma > 0; \quad u(0) = 0. \quad (134)$$

Weak formulation

$$\begin{cases} \text{Find } u \in H_{0,\omega}^1(\Lambda) \text{ such that} \\ a_\omega(u, v) = (f, v)_\omega, \quad \forall v \in H_{0,\omega}^1(\Lambda), \end{cases} \quad (135)$$

where $\omega := \omega_s^{\alpha,\beta}$, $H_{0,\omega}^1 = \{u \in H_\omega^1(\Lambda) : u(0) = 0\}$, and

$$a_\omega(u, v) = \gamma(u, v)_\omega + (\partial_x u, \partial_x(v\omega)), \quad \forall u, v \in H_{0,\omega}^1(\Lambda). \quad (136)$$

Denote $X_N = \{u \in V_{N,s}^{\alpha,\beta} : u(0) = 0\}$. Jacobi–Galerkin approximation is

$$\begin{cases} \text{Find } u_N \in X_N \text{ such that} \\ a_\omega(u_N, v_N) = (I_{N,s}^{\alpha,\beta} f, v_N)_\omega, \quad \forall v_N \in X_n, \end{cases} \quad (137)$$

Lemma 30. *Assume that*

$$d_1 = \max_{x \in \bar{\Lambda}} |\omega^{-1}(x) \partial_x \omega(x)|, \quad d_2 = \max_{x \in \bar{\Lambda}} |\omega^{-1}(x) \partial_x^2 \omega(x)|$$

are finite. Then, for any $u, v \in H_\omega^1(\Lambda)$,

$$a_\omega(u, v) \leq (d_1 + 1) \|u\|_{1, \omega} \|v\|_{1, \omega} + \gamma \|u\|_\omega \|v\|_\omega.$$

If, in addition $v^2(x) \omega'(x)|_{x=0}=0$ and $\lim_{x \rightarrow \infty} v^2 \omega'(x) \geq 0$, then

$$a_\omega(v, v) \geq \|v\|_{1, \omega}^2 + (\gamma - d_2/2) \|v\|_\omega^2, \quad \forall v \in H_\omega^1(\Lambda). \quad (138)$$

Theorem 31. *Assume that the condition of Lemma 30 are satisfied and $\gamma - d_2/2 > 0$. Then the problem (137) admits a unique solution. We have*

$$\|u - u_N\|_{1, \omega} \lesssim \inf_{v_N \in X_N} \|u - v_N\|_{1, \omega} + \|f - I_{N,s}^{\alpha, \beta} f\|_\omega. \quad (139)$$

For mapped Legendre method ($d_1 \leq 2, d_2 \leq 6$)

Corollary 32. *Let u and u_N be respectively the solution of (135) and (137) with $(\alpha, \beta) = (0, 0)$ and the mapping (110) with $s = 1$. Assume that $u \in \tilde{B}_{0,0}^m(\Lambda)$ and $f \in \tilde{B}_{0,0}^k(\Lambda)$, $k, m \geq 1$ and $\gamma > 3$, we have*

$$\|u - u_N\|_{1, \omega_1^{0,0}} \lesssim N^{1-m} \|D_x^m u\|_{\omega_1^{m,m}} + N^{-k} \|D_x^k f\|_{\omega_1^{k,k}}, \quad (140)$$

For mapped Chebyshev method. We have $d_1, d_2 = \infty$. but $a_\omega(\cdot, \cdot)$ is still continuous and coercive [cf. Guo et al. 2002].

Corollary 33. *Let u and u_N be the solution of (135) and (137) with $(\alpha, \beta) = (-1/2, -1/2)$ and the mapping (110) with $s = 1$. Assume that $u \in \tilde{B}_{-1/2, -1/2}^m(\Lambda)$ and $f \in \tilde{B}_{-1/2, -1/2}^m(\Lambda)$ and that $\gamma > \frac{14}{17}$, we have*

$$\begin{aligned} & \|u - u_N\|_{1, \omega_1^{-1/2, -1/2}} \\ & \lesssim N^{1-m} \|D_x^m u\|_{\omega_1^{m-1/2, m-1/2}} + N^{-k} \|D_x^k f\|_{\omega_1^{k-1/2, k-1/2}}, \end{aligned} \tag{141}$$

Implementation and Numerical Results

Take $\phi_k(x) = j_{s,k}^{0,0}(x) + j_{s,k+1}^{0,0}$ with $s = 1$ as basis of X_N ,
then $\omega(x) = \frac{2}{(1+x)^2}$.

(137) leads to a non-symmetric sparse system
(M tridiagonal, S seven diagonal)

$$(\gamma M + S)u = f \tag{142}$$

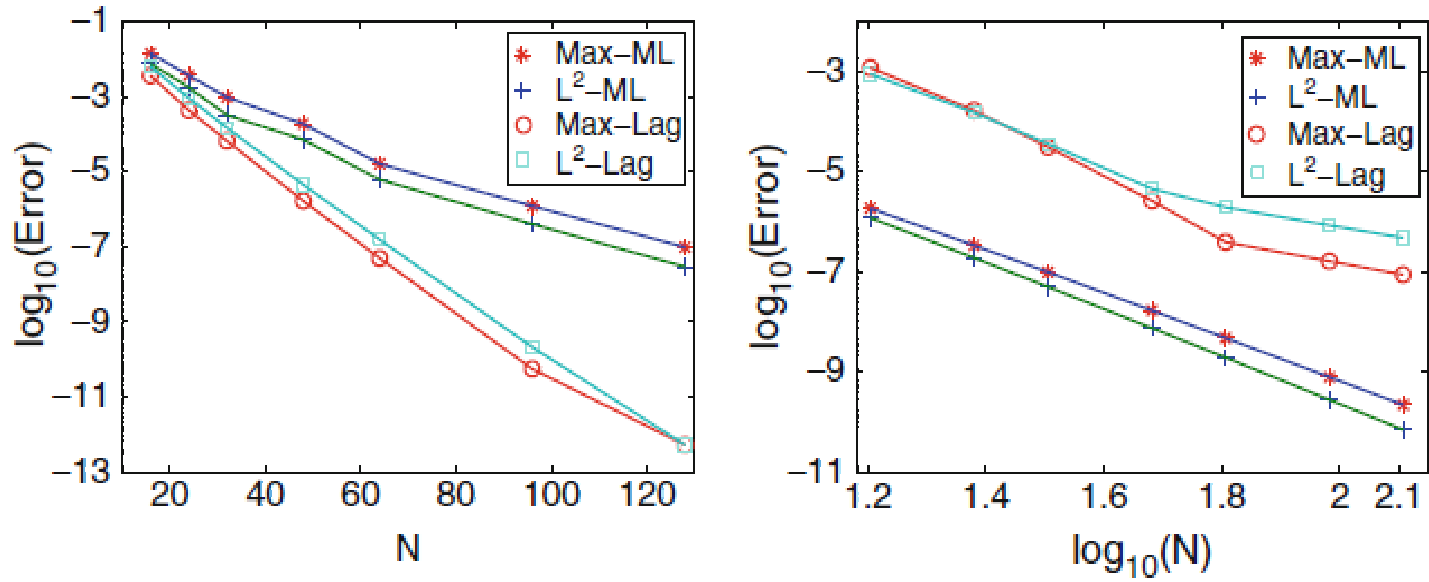


Figure 7. (Left) $u(x) = \sin(2x)e^{-x}$; (Right) $u(x) = 1/(1+x)^{5/2}$.

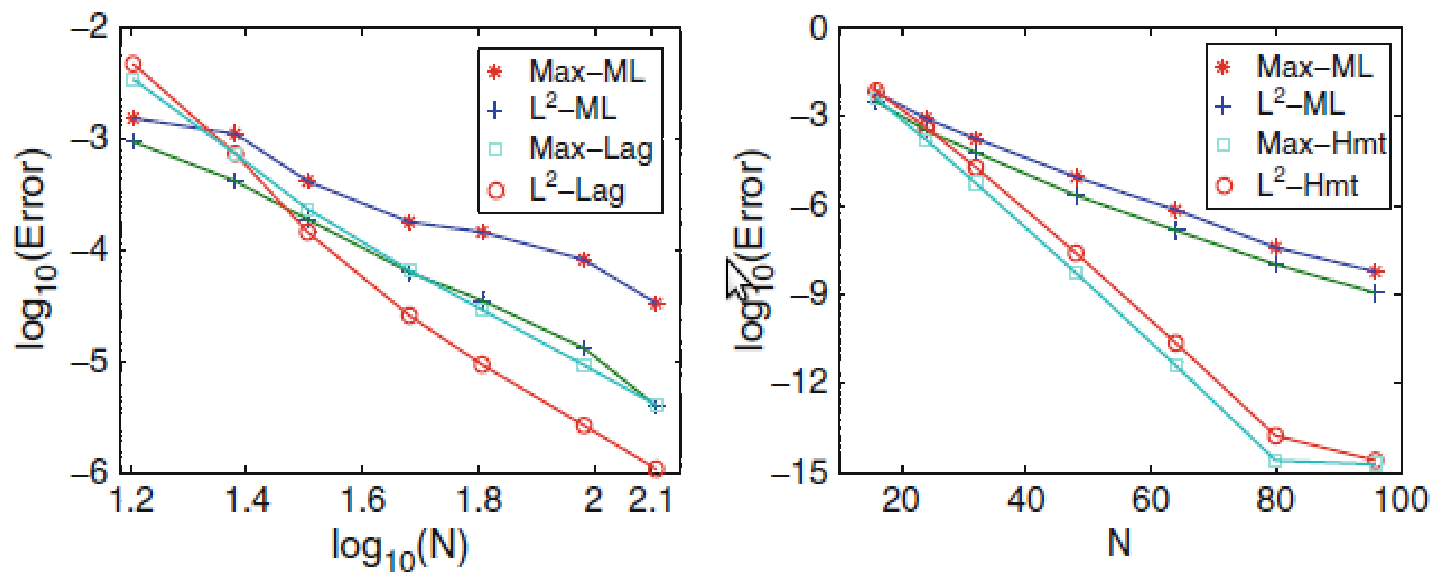


Figure 8. (Left) $u(x) = \sin(2x)/(1+x)^{7/2}$; (Right) $u(x) = \sin(2x)e^{-x^2}$.

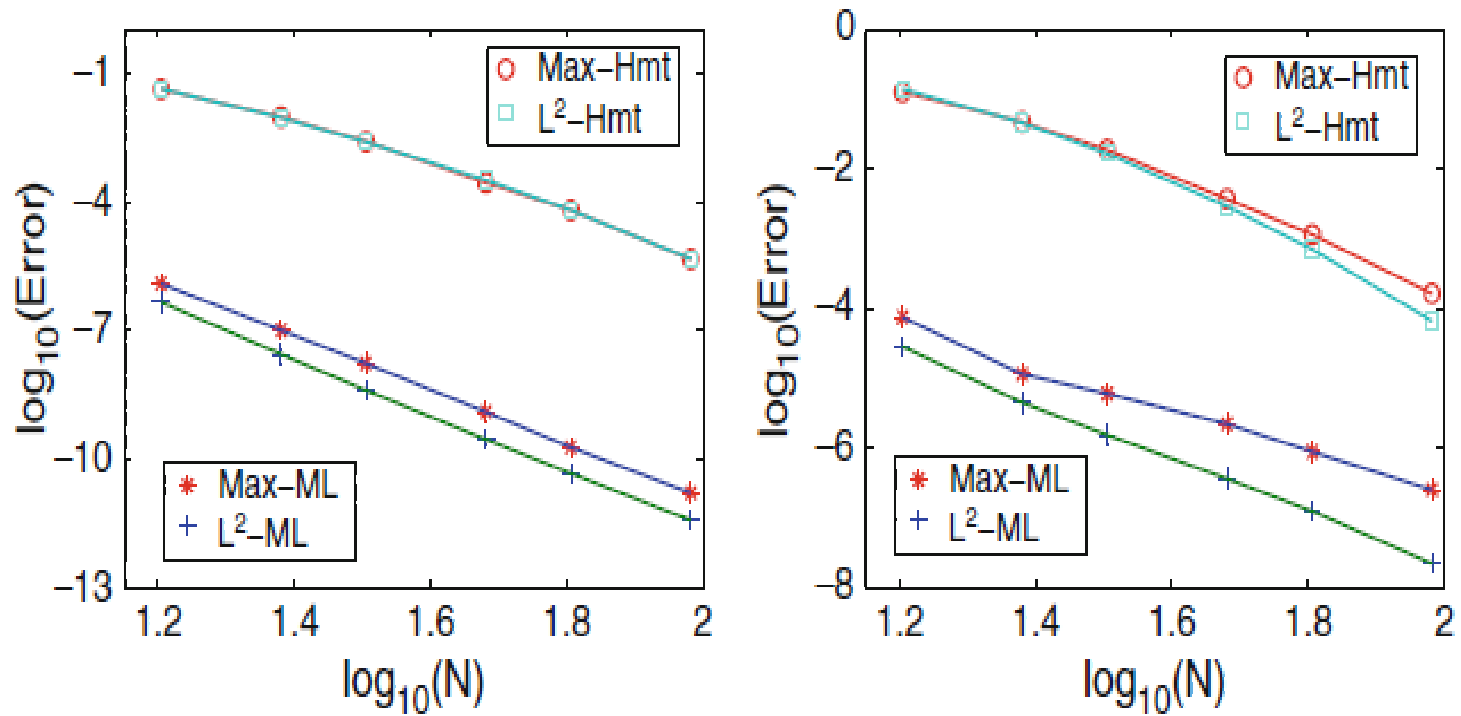


Figure 9. (Left) $u(x) = 1/(1+x^2)^{5/2}$; (Right) $u(x) = \sin(2x)/(1+x^2)^{7/2}$.

Conclusion

1. Two approaches to solve problem in unbounded domain
 - a. Laguerre/Hermite method
 - b. Mapped Jacobi method
2. The convergence rates of two approaches are compatible
3. Scaling parameter affects the convergence rates.