Recent advances in polynomial spectral approximations: Expansions and interpolation

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Polynomial spectral approximations

Let $\omega(x) \geq 0$ be a weight function on $\Omega := [a, b]$ and introduce

$$\langle f, g \rangle = \int_\Omega f(x)g(x)\omega(x)\mathrm{d}x.$$

Let $\{\phi_k\}_{k=0}^\infty$ denote the sequence of polynomials which are orthogonal with respect to $\langle \cdot, \cdot \rangle$ and $\langle \phi_k, \phi_j \rangle = \gamma_k \delta_{k,j}$.

Polynomial spectral approximations:

- **Expansion (i.e., Projection)**:

$$f_n(x) = \sum_{k=0}^n a_k \phi_k(x), \quad a_k = \frac{\langle f, \phi_k \rangle}{\gamma_k}.$$

- **Interpolation**:

$$p_n(x) = \sum_{j=0}^n f(x_j)\ell_j(x), \quad \ell_j(x) = \prod_{k \neq j} \frac{x - x_k}{x_j - x_k}.$$

Applications

- Spectral methods (Gottlieb & Orszag, 1977; Trefethen, 2000; Canuto, Hussaini, Quarteroni & Zang, 2006; Shen, Tang & Wang, 2011);
- Gauss, Fejér and Clenshaw-Curtis quadrature rules (Gauss, 1814; Fejér, 1933; Clenshaw & Curtis, 1960);
- Numerical inversion of Laplace transforms (Weeks, 1966);
- Rootfinding (Specht, 1960; Good, 1961; Day & Romero, 2005);
- Highly oscillatory integrals (Patterson, 1976; Domínguez, Graham & Smyshlyaev, 2011; Xiang, Cho, W. & Brunner, 2011);
- Convolutions (Hale & Townsend, 2014; Xu & Loureiro, 2018);
- $\cdots$

Why they are preferable?

Accuracy:

- Best or near-best approximations;
- Spectral accuracy.

Algorithm:

- FFT;
- Discrete polynomial transforms;
- Barycentric formula.

Myth 1. Best approximations are optimal

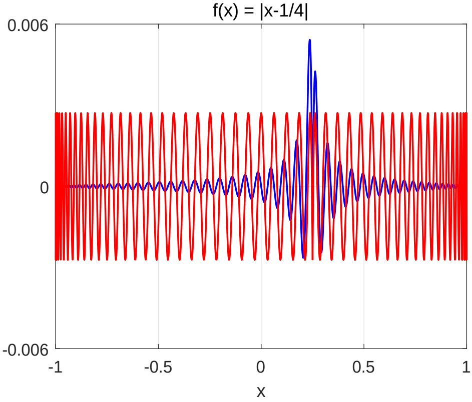

Figure 1: Pointwise error curves of p_n^{CC} (blue) and p_n^* (red) for $f(x) = |x - 1/4|$. Here $n = 100$.

Trefethen, Six myths of polynomial interpolation and quadrature, Maths. Today, 47:184-188, 2011.

Myth 2. Spectral approximations have exponential convergence

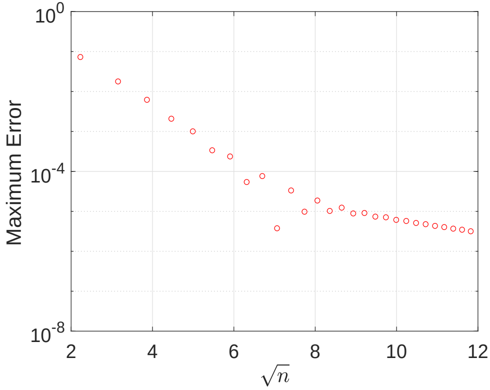

Figure 2: Maximum error of Laguerre expansion using $\{e^{-x/2}L_k(x)\}_{k=0}^n$ for $f(x) = 1/(1+x)^2$.

Shen & Wang, Some recent advances on spectral methods for unbounded domains, Commun. Comput. Phys., 5:195-241, 2009.

Lebesgue lemma

Lemma (DeVore & Lorentz, 1993)

Let X be a normed linear space and let Y be a finite-dimensional linear subspace of X. If L is a linear operator from X to Y which satisfies $Lf \equiv f$ for $f \in Y$. Then, for any $f \in X$, it holds that

$$\|f - Lf\| \leq (1 + \|L\|)E(f),$$

where $E(f) = \min_{g \in Y} \|f - g\|$ and $\|L\|$ is the Lebesgue constant.

Example. Consider the Gegenbauer expansion, i.e., $\phi_k(x) = C_k^{\lambda}(x)$, the Lebesgue constant satisfies (Frenzen & Wong, 1986)

$$\|L\|_{\infty} = \begin{cases} O(n^{\lambda}), & \lambda > 0, \\ O(\log n), & \lambda = 0. \\ O(1), & \lambda < 0. \end{cases}$$

Question: Do best approximations really converge faster than Gegenbauer expansions?

An example

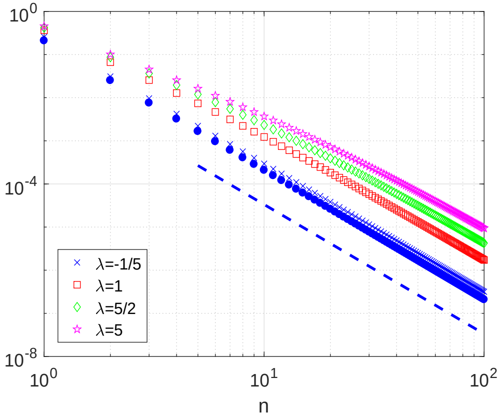

Figure 3: Maximum errors of best approximation (dots) and Gegenbauer expansion for $f(x) = (1+x)^{3/2}$. The dashed line is $O(n^{-3})$.

W., Optimal rates of convergence and error localization of Gegenbauer projections, IMA J. Numer. Anal., drac047, 2022.

Expansion coefficients

In recent years, a popular approach for developing error estimates of spectral expansions is

$$\|f-f_n\|_{L^2_\omega(\Omega)} = \sqrt{\sum_{k=n+1}^{\infty} |a_k|^2\gamma_k}, \ \ \|f-f_n\|_{L^\infty(\Omega)} \le \sum_{k=n+1}^{\infty} |a_k|\|\phi_k\|_\infty,$$

and the remaining issue is to find some sharp estimates for $\{a_k\}_{k=0}^{\infty}$.

Example. Consider the Legendre expansion, i.e., $\phi_k(x) = P_k(x)$. For $f(x) = |x|$, the Legendre coefficients satisfy (W. & Xiang, 2012; W., 2018; Xiang & Liu, 2020; Liu, Wang & Wu, 2021; W., 2023)

$$|a_k| \le \frac{4}{\sqrt{2\pi(k-1)}(k-1/2)} = O(k^{-3/2}), \quad k \ge 2.$$

Since $|P_k(x)| \le 1$, we obtain the maximum error bound

$$\|f-f_n\|_{L^\infty(\Omega)} \le \sum_{k=n+1}^{\infty} |a_k| \le \frac{8}{\sqrt{2\pi(n-1)}} = O(n^{-1/2}).$$

Is the rate $O(n^{-1/2})$ true?

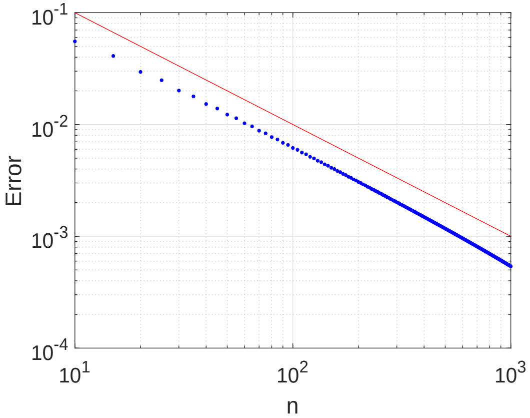

Figure 4: Log-log plot of $\|f - f_n\|_\infty$ (dots) for $f(x) = |x|$ and n^{-1} (line).

W., A new and sharper bound for Legendre expansion of differentiable functions, Appl. Math. Lett., 85:95–102, 2018.

Cauchy remainder for interpolation

The following theorem can be found in almost every textbook of numerical analysis.

Theorem

Let $f \in C^n(\Omega)$ and $f^{(n+1)}$ exists at each point of (a, b). Then, for each $x \in \Omega$, there exists $\xi = \xi(x) \in (a, b)$ such that

$$f(x) - p_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{j=0}^{n} (x - x_j).$$

Quotes

- "since the location of ξ in the interval $[a, b]$ is unknown, $\cdots$ is of little practical value" —— Süli & Mayers, 2004;
- "Unfortunately, the point ξ is unknown, so this result is not particularly useful unless we have a bound on the appropriate derivative of f" —— Heath, 2018.

Why and how

Why we need optimal error analysis?

- suboptimal error estimates may mislead us;
- understand spectral methods more accurately.

How to analyze optimal error estimates?

- Analytic functions;
- Differentiable functions.

Chebyshev expansion of analytic functions

Let $\mathcal{C}_\rho = \{z : |z| = \rho\}$ and let $\mathcal{E}_\rho$ denote the ellipse of the form

$$\mathcal{E}_\rho = \left\{ z : \; z = \frac{u + u^{-1}}{2}, \; u \in \mathcal{C}_\rho \right\}.$$

The Chebyhev expansion is

$$f_n(x) = {\sum_{k=0}^{n}}' a_k T_k(x), \quad a_k = \frac{2}{\pi} \int_{-1}^{1} \frac{f(x) T_k(x)}{\sqrt{1 - x^2}} \mathrm{d}x,$$

where the prime indicates that the first term of the sum is halved.

Theorem (Bernstein, 1912)

If f is analytic with $|f(z)| \leq M$ in the region bounded by the ellipse $\mathcal{E}_\rho$ for some $\rho > 1$, then for each $k \geq 0$,

$$a_k = \frac{1}{i\pi} \oint_{\mathcal{E}_\rho} \frac{f(z)}{u^k \sqrt{z^2 - 1}} \mathrm{d}z \quad \Longrightarrow \quad |a_k| \leq \frac{2M}{\rho^k}.$$

Note that optimal error estimates in L^2_ω and L^∞ can be derived!

Bernstein's idea

En effet, on a

$$f(x) = A_0 + A_1 T_1(x) + \cdots + A_n T_n(x) + \cdots,$$

où

$$A_n = \frac{1}{\pi} \int_0^{2\pi} f(\cos\theta) \cos n\theta d\theta,$$

et, en posant $e^{i\theta} = z$, on a

$$A_n = \frac{1}{2\pi i} \int_c f\left(\frac{z^2+1}{2z}\right) \cdot \frac{z^n + z^{-n}}{z} \cdot dz,$$

l'intégrale étant prise le long de la circonférence C de rayon 1.

Mais, par hypothèse, $f(x)$ est holomorphe à l'intérieur de l'ellipse E. Or, x décrit l'ellipse E, lorsque z parcourt le cercle de rayon R ou bien celui de rayon $\frac{1}{R}$ ayant le centre à l'origine, car

$$x = \frac{1}{2}\left(z + \frac{1}{z}\right) = \frac{1}{2}\left[\left(\Upsilon + \frac{1}{\Upsilon}\right)\cos\varphi + i\left(\Upsilon - \frac{1}{\Upsilon}\right)\sin\varphi\right],$$

en posant $z = \Upsilon e^{i\varphi}$. Donc, $f\left(\frac{z^2+1}{2z}\right)$ est holomorphe entre ces deux cercles,

Bernstein, Sur l'ordre de la meilleure approximation des fonctions continues par les polynômes de degré donné, Mem. Cl. Sci. Acad. Roy. Belg., 4:1–103, 1912.

Why Bernstein succeed?: $T_k(x) = (z^k + z^{-k})/2$.

Legendre expansion of analytic functions

Consider the Legendre expansion

$$f_n(x) = \sum_{k=0}^{n} a_k P_k(x), \quad a_k = \frac{2k+1}{2} \int_{-1}^{1} f(x) P_k(x) \mathrm{d}x.$$

Theorem (Iserles, 2011; W., 2016; W., 2021)

If f is analytic with $|f(z)| \le M$ in the region bounded by the ellipse $\mathcal{E}_\rho$ for some $\rho > 1$, then for each $k \ge 0$,

$$a_k = \frac{1}{i\pi} \oint_{\mathcal{E}_\rho} f(z) \left(\frac{c_k}{u^{k+1}} {}_2\mathrm{F}_1 \left[\begin{matrix} k+1, & \frac{1}{2}; \\ k+\frac{3}{2}; & \end{matrix} \ \frac{1}{u^2} \right] \right) \mathrm{d}z,$$

where $c_k = \Gamma(k+1)\Gamma(\frac{1}{2})/\Gamma(k+\frac{1}{2})$, it follows that

$$|a_0| \le \frac{D(\rho)}{2}, \quad |a_k| \le D(\rho) \frac{\sqrt{k}}{\rho^k}, \quad k \ge 1,$$

where $D(\rho) = 2ML/(\pi\sqrt{\rho^2 - 1})$.

A framework for expansions of analytic functions

Key idea:

1. Find the kernel $Q_k(z)$ such that
$$a_k = \oint_{\mathcal{C}} f(z) Q_k(z) \mathrm{d}z.$$
2. Choose appropriate $\mathcal{C}$ (i.e., boundary of the convergence domain).

A historical note:

The kernels were found in (Elliott & Tuan, 1974). Unfortunately, the contours $\mathcal{C}$ were chosen inappropriately and the authors failed to establish the optimal decay rate of a_k (Citation 15).

Recent advances:

- Gegenbauer (Cantero & Iserles, 2012; W., 2016; W., 2022);
- Jacobi (Xiang, 2012; Zhao, Wang & Xie, 2013);
- Laguerre (Elliott & Tuan, 1974; W., 2023).
- Hermite (Elliott & Tuan, 1974; Boyd, 1980; W. & Zhang, 2023).

Function spaces for differentiable functions

Key issue:

- Function spaces;
- Error localization.

Function spaces:

- AC-BV space (Trefethen, 2013):

$$\mathcal{W}^{\mu}(\Omega) = \left\{ f \;\middle|\; f, f', \ldots, f^{(\mu-1)} \in \mathrm{AC}(\Omega),\; f^{(\mu)} \in \mathrm{BV}(\Omega) \right\}.$$

- Fractional space (Liu, Wang & Li, 2019):

$$\mathbb{W}_{\theta}^{\mu+s}(\Omega) = \Big\{ f \;\Big|\; f, f', \ldots, f^{(\mu-1)} \in \mathrm{AC}(\Omega), \quad I_{\theta-}^{1-s} f^{(\mu)} \in \mathrm{BV}(\Omega_{\theta}^{-}), \quad I_{\theta+}^{1-s} f^{(\mu)} \in \mathrm{BV}(\Omega_{\theta}^{+}) \Big\},$$

where $\theta \in (-1, 1)$, $\Omega_{\theta}^{-} = (-1, \theta)$, $\Omega_{\theta}^{+} = (\theta, 1)$.

Example

For $f(x) = |x|$, $f \in C^0(\Omega)$, $f \notin C^1(\Omega)$, but $f \in \mathcal{W}^1(\Omega)$. For $f(x) = |x|^{3/2}$, then $f \in \mathbb{W}_{\theta}^{\mu+s}(\Omega)$ with $\theta = 0$, $\mu = 2$, $s = 1/2$.

Estimates of coefficients

Key idea:

- Rodrigues formula

Recent advances:

- Chebyshev
  - AC-BV space (Trefethen, 2008; Trefethen, 2013);
  - Fractional space (Liu, Wang & Li, 2019; Xie, Wu & Liu, 2023);
- Legendre
  - AC-BV space (W. & Xiang, 2012; W., 2018; W., 2023);
  - Fractional space (Liu, Wang & Wu, 2021);
- Jacobi
  - AC-BV space (Xiang & Liu, 2020).

Good news:

- Optimal error estimates in $L^2_\omega(\Omega)$;
- Optimal error estimates in $L^\infty(\Omega)$ for Chebyshev.

Why lost order?

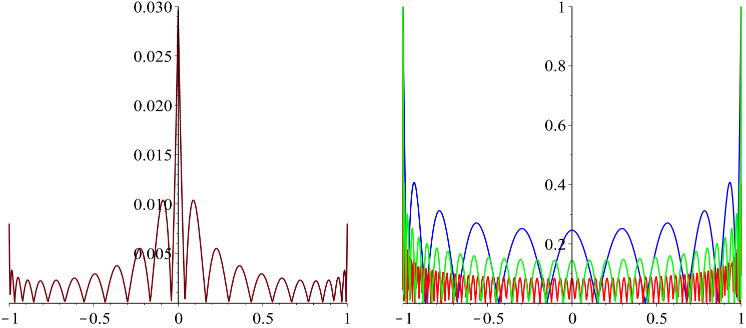

Figure 5: Pointwise error curve of Legendre expansion f_{20} for $f(x) = |x|$ (left) and $|P_k(x)|$ with $k = 10, 30, 90$.

Note that $|P_k(x)| = O(k^{-1/2})$ for $x \in (-1, 1)$ and $|P_k(\pm 1)| = 1$.

Error localization

For function with a singularity

$$f(x) = |x - \xi|^{\alpha} g(x),$$

where $\xi \in [-1, 1]$ and $\alpha > 0$ is not an even integer when $\xi \neq \pm 1$ and $\alpha > 0$ is not an integer when $\xi = \pm 1$.

Pointwise convergence rate: In the case $\xi \in (-1, 1)$, the pointwise error of Legendre projection is (W., 2023)

$$|f(x) - f_n(x)| = \begin{cases} O(n^{-\alpha-1}), & x \in (-1, \xi) \cup (\xi, 1), \\ O(n^{-\alpha-1/2}), & x = \pm 1, \\ O(n^{-\alpha}), & x = \xi. \end{cases}$$

Key ingredient:

$$\Psi_{\nu}^{\mathrm{C}}(x, n) = \sum_{k=n+1}^{\infty} \frac{\cos(kx)}{k^{\nu+1}}, \quad \Psi_{\nu}^{\mathrm{S}}(x, n) = \sum_{k=n+1}^{\infty} \frac{\sin(kx)}{k^{\nu+1}}.$$

where $\nu > -1$ if $x (\mathrm{mod}\ 2\pi) \neq 0$ and $\nu > 0$ if $x (\mathrm{mod}\ 2\pi) = 0$.

Interpolation of analytic functions

Theorem (Hermite, 1878)

If f is analytic inside in a simply connected region D containing the interval Ω, then

$$f(x) - p_n(x) = \frac{1}{2\pi i} \oint_{\mathcal{S}} \frac{\omega_n(x)}{\omega_n(z)} \frac{f(z)}{z-x} \mathrm{d}z,$$

where $\mathcal{S}$ is a simple closed curve that lies in D and contains the interval Ω and $\omega_n(x) = \prod_{k=0}^{n}(x - x_k)$.

By Hermite integral formula,

$$\|f - p_n\| \leq \max_{\substack{z\in\mathcal{S} \\ x\in\Omega}} \left| \frac{\omega_n(x)}{\omega_n(z)} \right| \frac{1}{2\pi} \oint_{\mathcal{S}} \frac{|f(z)|}{|z-x|} \mathrm{d}s,$$

and the convergence rate of p_n is determined by $|\omega_n(x)/\omega_n(z)|$ for $z \in \mathcal{S}$ and $x \in \Omega$.

Jacobi polynomials on ellipse

When $z \in \mathcal{E}_\rho$ for $\rho > 1$ (Kuijlaars, McLaughlin, Van Assche & Vanlessen, 2004)

$$P_n^{(\alpha,\beta)}(z) \cong \frac{2^{\alpha+\beta}}{\sqrt{\pi n}}(1-u^{-1})^{-\alpha-1/2}(1+u^{-1})^{-\beta-1/2}u^n$$

which implies that $|P_n^{(\alpha,\beta)}(z)| = O(\rho^n)$ for $z \in \mathcal{E}_\rho$.

Recent advances:

- Chebyshev interpolation (Reddy & Weideman, 2005);
- Gegenbauer interpolation (Xie, Wang & Zhao, 2013);
- Jacobi interpolation (Wang, Zhao & Zhang, 2014).

Interpolation of differentiable functions: The Chebyshev case

Theorem (Xiang, Chen & W., 2010; Trefethen, 2013)

If $f \in \mathcal{W}^{\mu}$ for some $\mu \in \mathbb{N}$, then for $n \geq \mu + 1$, the error of Chebyshev interpolants can be bounded by

$$\|f - p_n\|_{L^\infty(\Omega)} \leq \frac{4V_\mu}{\mu\pi} \prod_{j=1}^{\mu} \frac{1}{n+1-j}.$$

Key idea: Aliasing formula. For example, in the case of Chebyshev-Lobatto (i.e., Clenshaw-Curtis) points $x_j = \cos(j\pi/n)$,

$$c_k = a_k + \sum_{j=1}^{\infty} \left(a_{2jn-k} + a_{2jn+k}\right), \quad k = 0, \ldots, n,$$

where c_k is the Chebyshev coefficients of p_n.

Interpolation of differentiable functions

Theorem (Xiang, 2016)

If $f \in \mathcal{W}^{\mu}$ for some $\mu \in \mathbb{N}$, then for $n \geq \mu + 1$, the error of the interpolating polynomial p_n can be bounded by

$$\|f - p_n\|_{L^\infty(\Omega)} \leq \frac{\pi^{\mu} V_{\mu}}{(n-1)\cdots(n-\mu)} \max_{0 \leq j \leq n} \|\ell_j\|_{L^\infty(\Omega)},$$

where $\ell_j(x)$ are the Lagrange basis polynomials.

Key idea: Peano kernel theorem & Wainerman's lemma.

Remark

- It is a remarkable improvement for functions with interior singularities of integer order, i.e., $E(f) = O(n^{-\mu})$. In this case, the Lebesgue constant $\max_{x \in \Omega} \sum_{j=0}^{n} |\ell_j(x)|$ has been replaced by $\max_{0 \leq j \leq n} \|\ell_j\|_{L^\infty(\Omega)}$.
- When $\{x_j\}_{j=0}^{n}$ are strongly normal, then $\max_{0 \leq j \leq n} \|\ell_j\|_{L^\infty(\Omega)}$ is bounded, and therefore p_n converges at the rate $O(n^{-\mu})$.

Concluding remarks

Optimal error estimates of polynomial spectral approximations in $L^2_\omega(\Omega)$ and $L^\infty(\Omega)$ norms have experienced fast development in the past decade. These estimates will help us to understand more accurately the convergence behaviors of numerical methods that involve polynomial spectral approximations.

It is possible to extend these to other spectral approximations, such as

- Jacobi rational functions (Wang & Guo, 2007);
- Müntz polynomials (Hou, Lin, Azaiez & Xu, 2019);
- Mapped Chebyshev functions (Sheng, Shen, Tang, Wang & Yuan, 2020).

Thank you for your attention!