Math 6630: Numerical Solutions of Partial Differential Equations
Polynomial spectral methods, I

See Shen, Tang, and Wang 2011, Chapter 3,

Hesthaven, S. Gottlieb, and D. Gottlieb 2007, Chapters 4, 5

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Non-periodic problems

We have considered PDE's with periodic boundary conditions using Fourier Series.

Our main goal now is to modify our procedures appropriately for nonperiodic problems, e.g., ones of the form,

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Recall that to solve such (stationary) problems, we will essentially use Lax-Milgram and Céa's Lemma, which carry over directly to this case.

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The main tools we are lacking are

- Identification of a suitable (computationally convenient) basis
- Fundamental estimates for polynomial approximation of smooth functions
- Knowledge of an appropriate quadrature/interpolation grid

These are among the concepts we'll describe now (all in one spatial dimension).

Approximation with polynomials, I

There are handful of fundamental polynomial approximation estimates that we can exercise. We'll use some standard notation:

$$L^\infty(D) := \left\{ u : D \to \mathbb{R} \;\middle|\; \|u\|_{L^\infty} < \infty \right\}, \qquad \|u\|_{L^\infty} = \sup_{x \in D} |u(x)|.$$

$$C(D) := \{ u : D \to \mathbb{R} \;\; u \text{ is continuous on } D \}, \qquad P_n := \operatorname{span}\left\{ x^j \;\middle|\; 0 \leqslant j \leqslant n \right\}.$$

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Perhaps the most well-known polynomial approximation estimate is the following:

Theorem (Weierstrass)

Assume $u \in C([-1,1])$. Then given $\epsilon > 0$, there exists some $n \in \mathbb{N}$ and $p_n \in P_n$ such that

$$\|u - p_n\|_{L^\infty([-1,1])} \leqslant \epsilon.$$

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While the result above holds for more general intervals of $\mathbb{R}$, compactness of these intervals is essential. The result can be extended to infinite intervals through extra assumptions.

Theorem

Assume $u \in C([0,\infty))$ and that there is some $\delta > 0$ such that $\lim_{x\to\infty} u(x)e^{-\delta x} = 0$. Then for any $\epsilon > 0$, there exists some $n \in \mathbb{N}$ and $p_n \in P_n$ such that,

$(-\infty, \infty) \to e^{-\delta x^2}$

$$\left\| (u(x) - p_n(x)) e^{-\delta x} \right\|_{L^\infty([0,\infty))} < \epsilon.$$

Approximation with polynomials, II

Unfortunately, these estimation results are not constructive, and essentially rely on the ability to solve the (well-posed) problem,

$$p_n = \underset{p \in P_n}{\arg\min} \left\| u - p \right\|_{L^\infty},$$

which is quite difficult computationally.

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Perhaps unsurprisingly, things are easier in L^2-type spaces. We need to introduce relevant notation:

$$L^2_\omega(D) := \left\{ u : D \to \mathbb{R} \;\middle|\; \|u\|_{L^2_\omega(D)} < \infty \right\}, \quad \|u\|^2_{L^2_\omega(D)} := \langle u, u \rangle_{L^2_\omega(D)}, \quad \langle u, v \rangle_{L^2_\omega(D)} := \int_D u$$

where $\omega : D \to [0, \infty)$ is a non-negative weight function.

$$\langle u, v \rangle_{L^2_\omega(D)} = \int_D u(x)\, v(x)\, \omega(x)\, dx$$

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where $\omega : D \to [0, \infty)$ is a non-negative weight function.

Through essentially the same argument as we applied for Fourier Series, the optimization problem,

$$p_n = \underset{p \in P_n}{\arg\min} \|u - p\|_{L^2_\omega},$$

for $u \in L^2_\omega$ likewise has a unique solution, given by,

$$p_n = \sum_{j=0}^{n} \widehat{u}_j \phi_j(x), \qquad\qquad \widehat{u}_j := \langle u, \phi_j \rangle_{L^2_\omega},$$

where $\{\phi_j\}_j$ is an(y) L^2_ω-orthonormal basis for P_n.

Orthogonal polynomials

The above motivates that it would be quite useful to construct a polynomial analogue for the Fourier exponential basis e^{ijx}, i.e., to compute an orthogonal basis.

This is one of the main reasons to study orthogonal polynomials. (Though there are many other reasons as well.)

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The most straightforward way to define an orthogonal polynomial basis would be through a Gram-Schmidt type approach.

$$\{x^k\}_{k \geq 0} \longrightarrow \{p_k\}_{k \geq 0}$$

Recall we define $p_0(x) := 1/b_0$. Subsequently:

$$\widetilde{p}_k(x) = x^k - \sum_{j=0}^{k-1} \left\langle x^k, p_{\underset{j}{\cancel{j-1}}}(x) \right\rangle_{L^2_\omega} p_{\underset{j}{\cancel{j-1}}}, \qquad p_k = \frac{\widetilde{p}_k}{\|\widetilde{p}_k\|_{L^2_\omega}}, \qquad k \geqslant 1.$$

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At the very least this serves as a basic theoretical definition for the sequence $\{p_n\}_{n=0}^{\infty}$.

This is also generally the approach with the least practical relevance: this is very ill-conditioned.

To obtain better strategies we have to get (much) more technical.

The three-term recurrence, I

One of the most fundamentally important properties of orthogonal polynomials is also one of the most straightforward to prove.

Lemma (Three-term recurrence)

Suppose $\{p_n\}_{n \geqslant 0}$ *is a sequence of* L^2_ω*-orthonormal polynomials with* $n = \deg p_n$.[1] *Then there are constants* a_n *and* b_n *satisfying* $a_n \in \mathbb{R}$ *and* $b_n > 0$ *such that,*

$$x p_n = b_{n+1} p_{n+1} + a_n p_n + b_n p_{n-1}, \qquad\qquad n \geqslant 0,$$

where we define $p_{-1} \equiv 0$ *and* $p_0 \equiv 1/b_0$*, with* $b_0^2 = \int_D \omega(x) \mathrm{d}x$.

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Proof.

Fix n. We have that,

$$x p_n = \sum_{j=0}^{n+1} c_j p_j, \qquad\qquad c_j = \langle x p_n, p_j \rangle_{L^2_\omega}.$$

But for any $k < n-1$, then

$$c_k = \langle x p_n, p_k \rangle_{L^2_\omega} = \langle p_n, x p_k \rangle_{L^2_\omega} \stackrel{\deg(x p_k) < n}{=} 0.$$

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Proof.

This proves that there are constants a_n, b_n, and d_n such that,

$$x p_n = d_n p_{n+1} + a_n p_n + b_n p_{n-1}.$$

But we also have that $d_n = b_{n+1}$:

$$d_n = \langle x p_n, p_{n+1} \rangle = \langle x p_{n+1}, p_n \rangle = b_{n+1}.$$

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The three-term recurrence, II

$$xp_n = b_{n+1}p_{n+1} + a_n p_n + b_n p_{n-1}, \qquad\qquad n \geqslant 0,$$

I.e.,

$$p_{n+1} = \frac{1}{b_{n+1}}\left(x - a_n\right) p_n - \frac{b_n}{b_{n+1}} p_{n-1}.$$

From a computational standpoint, evaluating $p_n(x)$ through the recurrence above is <u>much</u> more stable than using Gram-Schmidt-type approaches.

Clearly $a_n = a_n(\omega)$ and $b_n = b_n(\omega)$, but we don't yet have a way to compute these coefficients.

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The converse of the three-term recurrence is also true: I.e., if a sequence of polynomials $\{p_n\}_{n\geqslant 0}$ satisfies the three-term recurrence above with $a_n \in \mathbb{R}$ and $b_n > 0$, then $\{p_n\}_n$ is a sequence that is orthonormal with respect to some positive-definite linear functional L. I.e., $L(p_k p_n) = \delta_{kn}$ and $L(p_n^2) > 0$.

This converse result is called Favard's Theorem.

The Christoffel-Darboux formula

A second fundamental property of orthogonal polynomials that is worth stating is the Christoffel-Darboux formula:

Theorem

If $\{p_n\}_{n \geqslant 0}$ is a sequence of orthonormal polynomials with recurrence coefficients a_n and b_n, then for every $n \geqslant 0$:

$$\sum_{k=0}^{n} p_k(x) p_k(y) = b_{n+1} \frac{p_{n+1}(x) p_n(y) - p_{n+1}(y) p_n(x)}{x - y}, \qquad x \neq y$$

$$\sum_{k=0}^{n} p_k^2(x) = b_{n+1} \left[p'_{n+1}(x) p_n(x) - p_{n+1}(x) p'_n(x) \right],$$

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$$K_{n+1} = \sum_{k=0}^{n} p_k(x) p_k(y) = b_{n+1} \frac{p_{n+1}(x) p_n(y) - p_{n+1}(y) p_n(x)}{x - y}, \qquad x \neq y$$

$$\sum_{k=0}^{n} p_k^2(x) = b_{n+1} \left[p_{n+1}'(x) p_n(x) - p_{n+1}(x) p_n'(x) \right],$$

The proof is induction on n.

This relation may seem like an oddity, but it allows us to derive very practically useful properties.

We won't discuss enough to reveal its direct utility, but to hint at the importance of the Christoffel-Darboux relation, note that $K_n(x,y) = \sum_{k=0}^{n-1} p_k(x) p_k(y)$ is a *reproducing kernel*:

$$\langle p(\cdot), K_n(\cdot, y) \rangle_{L^2_\omega} = p(y), \qquad p \in P_{n-1}$$

Quadrature

The next useful property of orthogonal polynomials is in obtaining useful quadrature formula. However, what is "useful"?

In the Fourier Series case, we took equidistant points x_j and uniform weights on $[0, 2\pi)$:

$$x_j = \frac{2\pi j}{(2N+1)}, \qquad\qquad w_j = \frac{2\pi}{2N+1}.$$

We showed that this choice of quadrature resulted in several nice properties (including stable interpolation).

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Recall that this quadrature satisfied,

$$\int_0^{2\pi} e^{ikx} \mathrm{d}x = \sum_{m=1}^{2N+1} w_m e^{ikx_m}, \qquad\qquad |k| < 2N+1$$

It turns out that this is the property, *accurate quadrature for as many basis functions as possible*, that made everything work out so nicely for Fourier Series.

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(One can also show that with only $2N+1$ points it's not possible to integrate exactly for $|k| \leqslant 2N+1$.)

Therefore, our first goal should be to devise polynomial quadrature with a similar goal: integrate as many polynomials as possible.

Polynomial quadrature, I

Given the quadrature rule,

$$\int_D p(x)\mathrm{d}x \approx \sum_{j=1}^{n} w_{\cancel{n}\,j}\, p(x_{\cancel{n}\,j}),$$

our goal is to make the above equality for all $p \in P_m$, where m should be as large as possible.

One way to do this is via direct moment matching, which results in a system of $\cancel{2n}$ $(m+1)$ nonlinear equations with $2n$ unknowns.

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One way to do this is via direct moment matching, which results in a system of $\cancel{2}n$ $(m+1)$ nonlinear equations with $2n$ unknowns.

Note that the nonlinearity enters in the dependence on x_j, and the dependence on w_j is only linear. Hence, the "hard" part of this is actually determining the nodes.

However, this is not a very practical way to proceed for even moderately large n. A more elegant strategy is as follows: First, the *node polynomial* associated to a quadrature rule is defined as,

$$d(x) := \prod_{j=1}^{n} (x - x_j)$$

Note that the node polynomial characterizes the "hard" part of the quadrature rule.

Polynomial quadrature, II

Our first fundamental result in polynomial quadrature rather precisely characterizes node polynomials for accurate quadrature rules.

Theorem (Jacobi)

Let $d(x) \in P_n$ be the node polynomial for an n-point quadrature rule with nodes $\{x_j\}_{j \in [n]}$. Let k be such that $0 \leqslant k \leqslant n$. Then the following two statements are equivalent:

- *There are quadrature weights $\{w_j\}_{j \in [n]}$ such that,*

$$\int_D p(x)\omega(x)\mathrm{d}x = \sum_{j=1}^{n} w_j p(x_j), \qquad \forall \;\; p \in P_{n+k-1}.$$

- *The node polynomial d satisfies,*

$$\langle d, p \rangle_{L^2_\omega} = 0, \qquad \forall \;\; p \in P_{k-1},$$

  which is called a quasi-orthogonality condition.

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Note: taking $k > n$ is not possible. Hence, the optimal quadrature rule is associated to $k = n$: n quadrature points exactly integrate polynomials up to degree $2n - 1$. This is called a Gauss(ian) quadrature rule.

Sketch of a portion of the proof

To see why the quasi-orthogonality condition,

$$\langle d, p \rangle_{L^2_\omega} = 0, \qquad\qquad \forall \;\; p \in P_{k-1},$$

implies a quadrature rule with a certain amount of exactness, note that any polynomial $p \in P_{n+k-1}$ can be written as,

$$p(x) = d(x) q(x) + r(x), \qquad\qquad q \in P_{k-1}, \qquad\qquad r \in P_{n-1},$$

where q and r are the (polynomial) quotient and remainder resulting from dividing p by d.

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Now let the quadrature weights $\{w_j\}_{j=1}^n$ be the interpolatory weights, i.e., the weights w_j corresponding to (i) interpolating a polynomial P_{n-1}, and (ii) exactly integatinng this interpolant. [2]

This then implies that,

$$\int_D p(x)\omega(x)\mathrm{d}x = \int_D d(x)q(x)\omega(x)\mathrm{d}x + \int_D r(x)\omega(x)\mathrm{d}x.$$

[2] That these weights exist requires unisolvence of polynomial interpolation.

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The proof is completed by noting that

- The first integral is exactly zero (quasi-orthogonality of $d(x)$), and the quadrature rule exactly integrates this because each x_j is a root of $d(x)$.
- The second integral is exactly integrated by the quadrature rule since $r \in P_{n-1}$.

[2] That these weights exist requires unisolvence of polynomial interpolation.

Zeros of orthogonal polynomials

$k = n \Rightarrow \langle d(x), q(x) \rangle = 0, \; q \in P_{n-1} \Rightarrow d(x)$: orthogonal poly.

We have learned that in order to develop quadrature rules that are as accurate as possible (Gaussian rules), we must find the roots of orthogonal polynomials.
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Zeros of orthogonal polynomials

We have learned that in order to develop quadrature rules that are as accurate as possible (Gaussian rules), we must find the roots of orthogonal polynomials.
(The weights are somewhat easier to obtain once we know the roots.)

Of course, such optimal quadrature rules require that the orthogonal polynomial p_n has exactly n simple roots (we needed this for interpolation unisolvence). We actually have a stronger, much better result.

Theorem

Let $\{p_n\}_{n \geqslant 0}$ be a sequence of orthogonal polynomials in $L^2_\omega(D)$, where D is an interval (possibly infinite) on the real line. Then for every n, p_n has exactly n simple roots inside D.

Proof idea: if p_n has $r < n$ real-valued roots $\{x_j\}_{j=1}^r$ in D, then $p_n \prod_{j=1}^r (x - x_j)$ is single-signed on D and so must have non-zero integral, but the integral must be zero since p_n is orthogonal to every polynomial of degree $r < n$. A similar argument allows one to conclude that the roots in D must be simple.

Weights for Gaussian quadrature

We have established that Gaussian quadrature is well-posed, i.e., that for any fixed $n \in \mathbb{N}$, the set of points $\{x_j\}_{j=1}^n = p_n^{-1}(0)$ are the (unique!) nodes that ensure,

$$\int_D p(x)\omega(x)\mathrm{d}x = \sum_{j=1}^n w_j p(x_j), \qquad\qquad \forall \ p \in P_{2n-1}.$$

The quadrature weights w_j are well-defined by interpolation unisolvence, but what are their values?

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Theorem

The n-point Gaussian quadrature weights are given by,

$$w_j = \frac{1}{K_n(x_j)}, > 0 \qquad\qquad K_n(x) = K_n(x,x) = \sum_{j=0}^{n-1} p_j^2(x)$$

Weights for Gaussian quadrature

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$$\int_D p(x)\omega(x)\mathrm{d}x = \sum_{j=1}^n w_j p(x_j), \qquad\qquad \forall \;\; p \in P_{2n-1}.$$

The quadrature weights w_j are well-defined by interpolation unisolvence, but what are their values?

Theorem

The n-point Gaussian quadrature weights are given by,

$$w_j = \frac{1}{K_n(x_j)}, \qquad\qquad K_n(x) = K_n(x,x) = \sum_{j=0}^{n-1} p_j^2(x)$$

Here is a linear algebraic proof: define

$$\boldsymbol{V} = \begin{pmatrix} | & | & & | \\ p_0(\boldsymbol{x}) & p_1(\boldsymbol{x}) & \cdots & p_{n-1}(\boldsymbol{x}) \\ | & | & & | \end{pmatrix}, \quad \boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \quad \boldsymbol{W} = \mathrm{diag}(w_1, \ldots, w_n)$$

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By direct matrix multiplication:

$$\boldsymbol{G} := \boldsymbol{V}^T \boldsymbol{W} \boldsymbol{V}, \qquad\qquad (\boldsymbol{G})_{\ell-1,k-1} = \sum_{j=1}^{n} w_j p_\ell(x_j) p_k(x_j).$$

Since $p_\ell p_k \in P_{2n-1}$, then exactness of the Gaussian quadrature rule implies,

$$\boldsymbol{G} = \boldsymbol{I} \quad \Longrightarrow \quad \boldsymbol{V}^T \boldsymbol{W} \boldsymbol{V} = \boldsymbol{I}$$

$V^+ \sqrt{W} \sqrt{W} V = I$

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If we assume the weights w_j are non-negative:

$$\boldsymbol{V}^T \boldsymbol{W} \boldsymbol{V} = \boldsymbol{I} \quad \Longrightarrow \quad \widetilde{\boldsymbol{V}} := \sqrt{\boldsymbol{W}}\boldsymbol{V} \text{ is unitary} \quad \Longrightarrow \quad \boldsymbol{V}\boldsymbol{V}^T = \boldsymbol{W}^{-1}$$

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Comparing diagonal entries of this final equality proves the result.

The matrix $\widetilde{\boldsymbol{V}}$ is unitary, and hence is the analogue of the DFT in the polynomial setting: a well-conditioned, isometric map between point values and expansion coefficients.

Gaussian quadrature

We have established that the quadrature rule,

$$\{x_j\}_{j=1}^n = p_n^{-1}(0), \qquad\qquad w_j = \frac{1}{K_n(x_j)},$$

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The following fundamental observation, excercising only the three-term recurrence, is key:

$$\begin{array}{ccccccccc}
xp_0 & = & a_0 p_0 & + & b_1 p_1 & & & & \\
xp_1 & = & b_1 p_0 & + & a_1 p_1 & + & b_2 p_2 & & \\
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If we truncate this at n rows and write in matrix-vector form:

$$x\boldsymbol{p}(x) = \boldsymbol{J}\boldsymbol{p}(x) + b_n p_n(x) \boldsymbol{e}_n, \qquad\qquad \boldsymbol{p}(x) = (p_0(x), \ldots, p_{n-1}(x))^T,$$

with $\boldsymbol{e}_n$ the unit vector with 1 in location n and zero elsewhere.

The Jacobi matrix

$$x\boldsymbol{p}(x) = \boldsymbol{J}\boldsymbol{p}(x) + b_n p_n(x)\boldsymbol{e}_n, \qquad \boldsymbol{p}(x) = (p_0(x), \ldots, p_{n-1}(x))^T,$$

The matrix $\boldsymbol{J}$ is called the Jacobi matrix:

$$\boldsymbol{J} := \begin{pmatrix} a_0 & b_1 & & & \\ b_1 & a_1 & b_2 & & \\ & b_2 & a_2 & b_3 & \\ & & \ddots & \ddots & \end{pmatrix}$$

Note that it is *symmetric*, *tridiagonal*, and depends *only* on the recurrence coefficients.

The Jacobi matrix

$p_n \propto d(x) = \prod_{j=1}^{n} (x - x_j), \quad \{x_j\}_j = p_n^{-1}(0)$

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What is relevant for us is the realization that:

$$p_n(x_0) = 0 \quad \Longleftrightarrow \quad \boldsymbol{J}\boldsymbol{p}(x_0) = x_0\boldsymbol{p}(x_0),$$

i.e.,

$$p_n^{-1}(0) = \lambda(\boldsymbol{J}),$$

where $\lambda(\boldsymbol{J})$ is the spectrum of $\boldsymbol{J}$.

The Jacobi matrix

$$\int_D p(x)\omega(x)\,dx \simeq \sum_{j=1}^{n} p(x_j)w_j$$

$$x\boldsymbol{p}(x) = \boldsymbol{J}\boldsymbol{p}(x) + b_n p_n(x)\boldsymbol{e}_n, \qquad \boldsymbol{p}(x) = (p_0(x), \ldots, p_{n-1}(x))^T,$$

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Something even better is true: since x_j is an eigenvalue of $\boldsymbol{J}$ with corresponding eigenvector $\boldsymbol{p}(x_j)$, then suppose

$$\boldsymbol{J}\boldsymbol{v} = x_j\boldsymbol{v}, \qquad \|\boldsymbol{v}\| = 1.$$

Then $w_j = \boldsymbol{v}_1$, the first component of $\boldsymbol{v}$.

Quadrature through linear algebra

In summary, the optimal (Gaussian) quadrature rule,

$$\int_D p(x)\omega(x)\mathrm{d}x = \sum_{j=1}^{n} w_j p(x_j), \qquad\qquad \forall \;\; p \in P_{2n-1}.$$

has nodes $\{x_j\}_{j=1}^n$ and weights $\{w_j\}_{j=1}^n$ that can be computed by,

$$\{x_j\}_{j=1}^n = p_n^{-1}(0) = \lambda(\boldsymbol{J}),$$

and if $\boldsymbol{V}$ is a matrix whose columns contain unit-norm eigenvectors for $\boldsymbol{J}$, then the weights w_j are the first row of $\boldsymbol{V}$ (first components of each eigenvector).

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Of particular note: all of this requires <u>only</u> the recurrence coefficients a_n, b_n.

Thus, in addition to (stable) evaluation of polynomials, the three-term recurrence gives us a direct procedure to compute optimal quadrature (which also serves as a stable interpolation grid).

Classical orthogonal polynomials

There is no explicit analytic expression for recurrence coefficients for a general weight $\omega(x)$.

But orthogonal polynomials associated to certain choices of $\omega(x)$ happen to be solutions to classical types of differential equations, and this connection allows explicit determination of the recurrence coefficients.

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We begin with a more general setting of *Sturm-Liouville* problems:

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left[Q(x)\omega(x)\frac{\mathrm{d}y}{\mathrm{d}x}\right] - \lambda\omega(x)y(x) = 0,$$

where

- $\omega(x)$ is a weight/density function,
- $Q(x)$ is an at-most quadratic polynomial related to the boundary conditions
- λ is a constant

The study of such differential equations (and their associated solutions $y(x)$) is rich and deep.

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- λ is a constant

The study of such differential equations (and their associated solutions $y(x)$) is rich and deep.

For special choices of ω, Q, the solutions to such equations are orthogonal polynomials, and such families of orthogonal polynomials are classical orthogonal polynomials.

Solutions as orthogonal polynomials

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left[Q(x)\omega(x)\frac{\mathrm{d}y}{\mathrm{d}x}\right] - \lambda\omega(x)y(x) = 0,$$

A non-trivial solution to this problem is a pair $(y(x), \lambda)$. The value of λ is a called an eigenvalue, since,

$$\mathcal{S}(y) = \lambda y, \qquad\qquad \mathcal{S}(y) := -\frac{1}{\omega(x)}\frac{\mathrm{d}}{\mathrm{d}x}\left[Q(x)\omega(x)\frac{\mathrm{d}y}{\mathrm{d}x}\right].$$

Note in particular that $\mathcal{S}$ (with appropriate boundary conditions) is a self-adjoint operator: $\mathcal{S} = \mathcal{S}*$.

In addition $\mathcal{S}$ is positive semi-definite, so the eigenvalues λ are positive. (or 0)

These facts (with some additional technical details) implies that two linearly independent solutions are orthogonal in L^2_ω (and are complete in the same space).

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These facts (with some additional technical details) implies that two linearly independent solutions are orthogonal in L^2_ω (and are complete in the same space).

Of interest to us is that special choices of Q an ω lead to polynomial solutions, hence they are L^2_ω-orthogonal polynomials: $\{p_n, \lambda_n\}_{n=0}^\infty$.

Rodrigues' formula

One particularly powerful consequence of Sturm-Liouville theory occurs if we assume that ω satisfies the following *Pearson differential equation*:

$$\omega'(x) = \frac{L(x)}{Q(x)}\omega(x),$$

where $L(x)$ is an at-most linear polynomial.

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$$\omega'(x) = \frac{L(x)}{Q(x)}\omega(x),$$

where $L(x)$ is an at-most linear polynomial.

When this is the case and we have polynomial solutions p_n, then the Sturm-Liouville equation implies the following somewhat explicit formula for orthogonal polynomials, called Rodrigues' formula:

$$p_n(x) \propto \frac{1}{\omega(x)} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \left[Q(x)^n \omega(x)\right].$$

This formula, and its subsequent manipulation, allows explicit computation of the recurrence coefficients a_n, b_n.

Examples

At long last, here are some examples of classical orthogonal polynomial families:

Example (Legendre polynomials)

Take $\omega(x) \equiv 1$ for $x \in [-1, 1]$.

Define $Q(x) = (1 - x)(1 + x) = (1 - x^2)$.

Then $\{p_n\}_{n \geqslant 0}$ satisfy a Sturm-Liouville equation with eigenvalues,

$$\mathcal{S} p_n = \lambda_n p_n, \qquad\qquad \lambda_n = n(n+1) \sim n^2.$$

There is also a Rodrigues' formula, and the recurrence coefficients are for $n > 0$:

$$b_0 = \frac{1}{\sqrt{2}}, \qquad\qquad a_n = 0, \qquad\qquad b_n = \frac{n}{\sqrt{4n^2 - 1}}$$

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Example (Hermite polynomials)

Take $\omega(x) = e^{-x^2}$ for $x \in \mathbb{R}$.

Define $Q(x) = 1$.

Then $\{p_n\}_{n \geqslant 0}$ satisfy a Sturm-Liouville equation with eigenvalues,

$$\mathcal{S} p_n = \lambda_n p_n, \qquad \lambda_n = 2n$$

There is also a Rodrigues' formula, and the recurrence coefficients are for $n > 0$:

$$b_0 = \frac{1}{\pi^{1/4}}, \qquad a_n = 0, \qquad b_n = \sqrt{\frac{n}{2}}.$$

$$w'(x) = -2x\, e^{-x^2} = -2x\, w(x)$$

$$= \frac{-2x}{1} \cdot w(x)$$

Examples

At long last, here are some examples of classical orthogonal polynomial families:

Example (Chebyshev polynomials)

Take $\omega(x) = (1 - x^2)^{-1/2}$ for $x \in (-1, 1)$.

Define $Q(x) = (1 - x^2)$.

Then $\{p_n\}_{n \geqslant 0}$ satisfy a Sturm-Liouville equation with eigenvalues,

$$\mathcal{S} p_n = \lambda_n p_n, \qquad \lambda_n = n^2$$

Again, Rodrigues' formula provides explicit recurrence coefficients.

It is also well-known that $p_n(x) \propto \cos(n \arccos x)$, and this connection furnishes many useful properties, perhaps the most useful that forward- and inverse- interpolation problems with Chebyshev polynomials can be written in terms of the DFT, and hence can be accomplished with the fast Fourier transform.

Examples

At long last, here are some examples of classical orthogonal polynomial families:

Example (Jacobi polynomials)

This family generalizes Legendre and Chebyshev polynomials.

Take $\omega(x) = (1-x)^{\alpha}(1+x)^{\beta}$ for $x \in (-1,1)$ and any fixed $\alpha, \beta > -1$.

Define $Q(x) = (1-x^2)$.

Then $\{p_n\}_{n \geqslant 0}$ satisfy a Sturm-Liouville equation with eigenvalues,

$$\mathcal{S} p_n = \lambda_n p_n, \qquad\qquad \lambda_n = n(n+\alpha+\beta+1)$$

Again, Rodrigues' formula provides explicit recurrence coefficients.

Examples

At long last, here are some examples of classical orthogonal polynomial families:

Example (Laguerre polynomials)

Take $\omega(x) = x^\alpha e^{-x}$ for $x \in (0, \infty)$ and any fixed $\alpha > -1$.

Define $Q(x) = x$.

Then $\{p_n\}_{n \geqslant 0}$ satisfy a Sturm-Liouville equation with eigenvalues,

$$\mathcal{S} p_n = \lambda_n p_n, \qquad\qquad \lambda_n = n$$

Again, Rodrigues' formula provides explicit recurrence coefficients.

Approximation with polynomials

We have covered some practical mechanics with orthogonal polynomials, in particular: generation and quadrature, all of which boil down to knowing and manipulating recurrence coefficients.

Back to our aim of solving differential equations: are there approximation estimates?

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The precise details are far more technical than with Fourier Series, but the basic idea can be described without these details.

We'll describe the idea through an analogy: we showed one strategy to derive approximation estimates with Fourier Series, but here is an alternative, essentially equivalent method:

Consider the differential equation/eigenvalue problem,

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} y(x) = \lambda y(x),$$

with periodic boundary conditions. Let us use the notation:

$$\mathcal{S}(y) = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} y.$$

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$$\mathcal{S}(y) = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} y.$$

It is not difficult to see that,

$$\mathcal{S}(\phi_n) = \lambda_n \phi_n, \qquad \phi_n(x) = \frac{1}{\sqrt{2\pi}} e^{inx}, \qquad \lambda_n = n^2$$

Fourier Series, revisited

To compute error estimates for Fourier Series approximation, we defined the L^2-orthogonal projection coefficients for a function u:

$$\widehat{u}_n = \langle u, \phi_n \rangle,$$

and with orthonormality and completeness of ϕ_n, we computed a bound on the tail sum,

$$\sum_{n>N} |\widehat{u}_n|^2,$$

by directly estimating how fast $|\widehat{u}_n|$ decays with n.

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Here is a way to do this, where we hide details surrounding boundary condition enforcement.

First observe that $\mathcal{S}$ is self-adjoint through integration by parts:

$$\left\langle S(u), \phi_n \right\rangle = \left\langle u, \mathcal{S}(\phi_n) \right\rangle.$$

Then we have:

$$\begin{aligned} |\widehat{u}_n| = \left|\left\langle u, \phi_n \right\rangle\right| = \frac{1}{\lambda_n} \left|\left\langle u, \lambda_n \phi_n \right\rangle\right| = \frac{1}{\lambda_n} \left|\left\langle u, \mathcal{S}(\phi_n) \right\rangle\right| &= \frac{1}{\lambda_n} \left|\left\langle \mathcal{S}(u), \phi_n \right\rangle\right| \\ &= \frac{1}{\lambda_n} \left|\left\langle u''(x), \phi_n \right\rangle\right| \\ &= \frac{1}{\lambda_n} \left|\widehat{(u'')}_n\right| \end{aligned}$$

Fourier Series, revisited

Thus, we have

$\lambda_n = n^2$

$$|\hat{u}_n| = \frac{1}{\lambda_n} \left| \widehat{(u'')}_n \right|,$$

and so using that $\lambda_{n+1} > \lambda_n$ along with Parseval's equality,

$$\sum_{n>N} |\hat{u}_n|^2 \lesssim \frac{1}{\lambda_N^2} \|u''\|_{L^2}^2$$

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In other words, we can repeatedly use this trick of multiplying and dividing by λ_n to show that if $u \in H_p^{2s}$, then

$$\sum_{n>N} |\widehat{u}_n|^2 \lesssim \frac{1}{\lambda_N^{2s}} \|u^{(2s)}\|_{L^2}^2,$$

i.e.,

$$\|u - u_N\|_{L^2} \lesssim \frac{1}{\lambda_N^s} \|u\|_{H^{2s}} \sim N^{-2s} \|u\|_{H^{2s}},$$

which is exactly what we concluded before.

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which is exactly what we concluded before.

The difference now: this works almost exactly the same way for polynomial approximation.

Polynomial approximation via Sturm-Liouville theory

Therefore, note that with $\mathcal{S}(p_n) = \lambda_n p_n$ our Sturm-Liouville eigenpairs, then we have essentially the same argument:

$$\left|\langle u, p_n \rangle\right| = \frac{1}{\lambda_n} \left|\langle u, \mathcal{S}(p_n) \rangle\right| = \frac{1}{\lambda_n} \left|\langle \mathcal{S}(u), p_n \rangle\right|.$$

Note the difference here is that $\mathcal{S}(u)$ is not the standard second differentiation operator. Therefore, one needs special kinds of norms to properly articulate estimates.

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Note the difference here is that $\mathcal{S}(u)$ is not the standard second differentiation operator. Therefore, one needs special kinds of norms to properly articulate estimates.

For example, for Legendre polynomial approximation ($\omega(x) = 1$ for $x \in [-1, 1]$), define,

$$\widetilde{H}^s := \left\{ u \in L^2([-1,1]) \;\middle|\; u^{(j)} \in L^2_{Q^j}, \;\; j = 1, \ldots, s \right\},$$

where $Q(x) = 1 - x^2$. Then if $u \in \widetilde{H}^s$,

$$\|u - \mathcal{P}_N u\|_{L^2} \lesssim N^{-s} \|u^{(s)}\|_{L^2_{Q^s}}, \quad \sim N^{-s} \|u\|_{\widetilde{H}^s}$$

where $\mathcal{P}_N$ is the L^2-orthogonal projection onto degree-N polynomials, P_N.

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Therefore, note that with $\mathcal{S}(p_n) = \lambda_n p_n$ our Sturm-Liouville eigenpairs, then we have essentially the same argument:

$$|\langle u, p_n \rangle| = \frac{1}{\lambda_n} |\langle u, \mathcal{S}(p_n) \rangle| = \frac{1}{\lambda_n} |\langle \mathcal{S}(u), p_n \rangle| .$$

Note the difference here is that $\mathcal{S}(u)$ is not the standard second differentiation operator. Therefore, one needs special kinds of norms to properly articulate estimates.

For example, for Legendre polynomial approximation ($\omega(x) = 1$ for $x \in [-1, 1]$), define,

$$\widetilde{H}^s := \left\{ u \in L^2([-1,1]) \;\middle|\; u^{(j)} \in L^2_{Q^j}, \;\; j = 1, \ldots, s \right\},$$

where $Q(x) = 1 - x^2$. Then if $u \in \widetilde{H}^s$,

$$\|u - \mathcal{P}_N u\|_{L^2} \lesssim N^{-s} \|u^{(s)}\|_{L^2_{Q^s}},$$

where $\mathcal{P}_N$ is the L^2-orthogonal projection onto degree-N polynomials, P_N.

Of special note is that for polynomial methods, one does *not* in general obtain the optimal convergence rates for measuring errors of higher derivatives.

Spectral methods

$$\|u - \mathcal{P}_N u\|_{L^2} \lesssim N^{-s} \|u^{(s)}\|_{L^2_{Q^s}},$$

Note that N^{-s} dependence, more explicity written out comes from the fact that,

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Hence, the rate of approximation comes entirely from the regularity of u and the asymptotic behavior of the spectrum of the Sturm-Liouville operator $\mathcal{S}$.

Approximation schemes (especially in the context of differential equations) whose approximation rates have such an origin are called spectral methods.

On to differential equations

We have provided concrete answers to the following challenges we pointed out at the beginning of this discussion:

- Identification of a suitable (computationally convenient) basis (orthogonal polynomials)
- Fundamental estimates for polynomial approximation of smooth functions (spectral method estimates)
- Knowledge of an appropriate quadrature/interpolation grid (Gaussian quadrature)

Our next goal is to exercise these tools for solving differential equations.

References I

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