

1 Chapter 4: orthogonal polynomial methods for differential equations

Here we discuss

1. The de
2. The solution of 2-point boundary value problems with four methods: ultraspherical method, collocation method, finite difference method, the ultraspherical method in weak form. Prove convergence of the finite difference method
3. Next chapter: finite difference methods for time-dependent PDEs
4. We must do two-dimensional PDEs

In the previous chapter, we learnt that interpolants expressed in terms of Chebyshev polynomials can be very useful for approximating non-periodic functions. We learnt that there are fast algorithms for computing Chebyshev interpolants and their derivatives and these can be used to approximate solutions to PDEs.

Chebyshev polynomials are examples of *orthogonal polynomials* (OPs). In this chapter we'll learn that OPs can be used to design *sparse* methods for differential equations.

OPs are fundamental for computational mathematics, with applications in function approximation, quadrature (calculating integrals), solving differential equations, spectral analysis of Schrödinger operators, etc. In addition, OPs play a very important role in many mathematical areas including representation theory, functional analysis, integrable systems, singular integral equations, complex analysis, and random matrix theory.

Note: In previous chapters, a polynomial $p_n(x)$ denoted an interpolating polynomial through n distinct nodes and p_n had degree $\leq n - 1$. In this chapter, unless stated otherwise, $p_n(x)$ denotes a polynomial of degree precisely n , i.e.,

$$p_n(x) = k_n x^n + \mathcal{O}(x^{n-1})$$

where $k_n \neq 0$.

The set of polynomials of degree $\leq n$ with real coefficients, \mathbb{P}_n , is a linear space (or vector space) of dimension $n + 1$. The set of monomials of degree $\leq n$, $\{1, x, x^2, \dots, x^n\}$, is a basis for the space \mathbb{P}_n , meaning that all polynomials of degree $\leq n$ can be expressed as linear combinations of monomials. Likewise, $\{p_0(x), p_1(x), \dots, p_n(x)\}$ is a basis of \mathbb{P}_n . It is much more efficient and stable to perform computations in OP bases as opposed to the monomial basis.

1.1 Definition of orthogonal polynomials

Let $p_0(x), p_1(x), p_2(x), \dots$ be a sequence of polynomials such that $p_n(x)$ is exactly of degree n , i.e., $p_n(x) = k_n x^n + \mathcal{O}(x^{n-1})$ where $k_n \neq 0$. Let $w(x)$ be a continuous weight function on a (possibly infinite) interval (a, b) : that is $w(x) \geq 0$ for all $a < x < b$. This induces an inner product

$$\langle f, g \rangle := \int_a^b f(x)g(x)w(x)dx$$

We say that $\{p_0, p_1, \dots\}$ are *orthogonal with respect to the weight w* if

$$\langle p_n, p_m \rangle = 0 \quad \text{for } n \neq m.$$

Because w is continuous, we have

$$\|p_n\|^2 = \langle p_n, p_n \rangle > 0.$$

Orthogonal polynomials are not unique: we can multiply each p_n by a different nonzero constant $\tilde{p}_n(x) = c_n p_n(x)$, and \tilde{p}_n will be orthogonal w.r.t. w . However, if we specify k_n , this is sufficient to uniquely define them:

Proposition (Uniqueness of OPs) Given a non-zero k_n , there is a unique polynomial p_n orthogonal w.r.t. w to all lower degree polynomials.

Proof Suppose $r_n(x) = k_n x^n + O(x^{n-1})$ is another OP w.r.t. w . We want to show $p_n - r_n$ is zero. But this is a polynomial of degree $< n$, hence

$$p_n(x) - r_n(x) = \sum_{k=0}^{n-1} c_k p_k(x)$$

But we have for $j \leq n-1$

$$\langle p_j, p_j \rangle c_j = \langle p_n - r_n, p_j \rangle = \langle p_n, p_j \rangle - \langle r_n, p_j \rangle = 0 - 0 = 0$$

which shows all c_j are zero. Note that we used the linearity property of the inner product: for constants α, β and functions $f(x), g(x)$ and $h(x)$, it follows that $\langle f, \alpha g + \beta h \rangle = \alpha \langle f, g \rangle + \beta \langle f, h \rangle$. ■

Corollary If q_n and p_n are orthogonal w.r.t. w to all lower degree polynomials, then $q_n(x) = C p_n(x)$ for some constant C .

Example and Proposition (Chebyshev polynomials of the first kind are OPs) The Chebyshev polynomials of the first kind,

$$T_n(x) = \cos n \arccos x,$$

are OPs on $x \in [-1, 1]$ with respect to the weight

$$w(x) = \frac{1}{\sqrt{1-x^2}},$$

and

$$k_0 = 1, \quad k_n = 2^{n-1}, \quad n \geq 1.$$

Proof It follows immediately from the definition that $T_0(x) = 1$, $T_1(x) = x$ and for $n \geq 1$, setting $x = \cos \theta$,

$$xT_n(x) = \cos \theta \cos n\theta = \frac{\cos(n-1)\theta + \cos(n+1)\theta}{2} = \frac{T_{n-1}(x) + T_{n+1}(x)}{2}$$

In other words $T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$ for $n \geq 1$. This shows that $T_n(x) = k_n x^n + \mathcal{O}(x^{n-1})$ with $k_0 = 1$ and $k_n = 2^{n-1}$, $n \geq 1$. What remains to be shown is orthogonality with respect to the inner product defined by $w(x)$: again setting $x = \cos \theta$

$$\begin{aligned}\langle T_n, T_m \rangle &= \int_{-1}^1 \frac{T_n(x)T_m(x)}{\sqrt{1-x^2}} dx \\ &= \int_0^\pi \cos n\theta \cos m\theta dx \\ &= \begin{cases} 0 & \text{if } n \neq m \\ \frac{\pi}{2} & \text{if } n = m \geq 1, \\ \pi & \text{if } n = m = 0 \end{cases}\end{aligned}$$

which completes the proof. ■

1.1.1 Monic orthogonal polynomials

If $k_n = 1$, that is,

$$p_n(x) = x^n + O(x^{n-1})$$

then we refer to the orthogonal polynomials as monic.

Monic OPs are unique as we have specified k_n .

1.1.2 Orthonormal polynomials

If $\|p_n\| = 1$, then we refer to the orthogonal polynomials as orthonormal w.r.t. w . We will usually use q_n when they are orthonormal. Note they're not unique: we can multiply by ± 1 without changing the norm.

Proposition (existence) Given a weight $w(x)$, monic orthogonal polynomials exist.

Proof Existence follows immediately from the GramSchmidt procedure. That is, define $p_0(x) := 1$ and

$$p_n(x) := x^n - \sum_{k=0}^{n-1} \frac{\langle x^n, p_k \rangle}{\|p_k\|^2} p_k(x)$$

■

1.2 Function approximation with OPs

A basic usage of orthogonal polynomials is for approximating functions. First we observe the following:

Proposition (expansion) If $f(x)$ is a degree n polynomial, $\{p_n\}$ are orthogonal and $\{q_n\}$ are orthonormal then

$$\begin{aligned}
f(x) &= \sum_{k=0}^n \frac{\langle p_k, f \rangle}{\|p_k\|^2} p_k(x) \\
&= \sum_{k=0}^n \langle q_k, f \rangle q_k(x)
\end{aligned}$$

Proof Because $\{p_0, \dots, p_n\}$ are a basis of the space of polynomials of degree $\leq n$, we can write

$$f(x) = \sum_{k=0}^n f_k p_k(x)$$

for constants $f_k \in \mathbb{R}$. By linearity we have

$$\langle p_m, f \rangle = \sum_{k=0}^n f_k \langle p_m, p_k \rangle = f_m \langle p_m, p_m \rangle$$

for $m = 0, \dots, n$, i.e.,

$$f_k = \frac{\langle p_k, f \rangle}{\langle p_k, p_k \rangle}, \quad k = 0, \dots, n.$$

■

If f is not a polynomial, we make the approximation $f(x) \approx \sum_{k=0}^n f_k p_k(x)$, with the expansion coefficients f_k defined as above.

Example: For Chebyshev polynomials, $p_k(x) = T_k(x)$ and for $k \geq 1$,

$$\begin{aligned}
f_k &= \frac{\langle T_k, f \rangle}{\langle T_k, T_k \rangle} = \frac{\langle T_k, f \rangle}{\|T_k\|^2} \\
&= \frac{2}{\pi} \int_{-1}^1 \frac{f(x) T_k(x)}{\sqrt{1-x^2}} dx \\
&= \frac{2}{\pi} \int_0^\pi f(\cos \theta) \cos k\theta d\theta \\
&= \frac{1}{\pi} \int_{-\pi}^\pi f(\cos \theta) \cos k\theta d\theta \\
&= \frac{1}{\pi} \int_{-\pi}^\pi f(\cos \theta) e^{-ik\theta} d\theta \\
&= \frac{(-1)^k}{\pi} \int_0^{2\pi} f(\cos(\theta - \pi)) e^{-ik\theta} d\theta
\end{aligned}$$

That is, for Chebyshev polynomials, the expansion coefficients f_k (aka Chebyshev coefficients) can be expressed as Fourier coefficients and therefore, they can be approximated with the FFT, as we learned in Chapter 3.

1.3 Three-term recurrences and Jacobi matrices for general orthogonal polynomials

1.3.1 Three-term recurrence relationships

In Chapter 3, we used the formula $T_n(x) = \cos n \arccos x$ and trigonometric identities to show that the Chebyshev polynomials satisfy a three-term recurrence relationship: $T_0(x) = 1$, $T_1(x) = x$ and for $n \geq 1$,

$$xT_n(x) = \frac{1}{2}T_{n-1}(x) + \frac{1}{2}T_{n+1}(x).$$

We'll soon prove that, as a consequence of orthogonality, all OP families satisfy three-term recurrences, which is a fundamental property of OPs. By collecting OPs in a vector, we'll see that three-term recurrences can be expressed as multiplication by a tridiagonal matrix, the Jacobi matrix associated with a family of OPs.

A central theme: if you know the Jacobi matrix / three-term recurrence, you know the polynomials. This is the **best** way to evaluate expansions in orthogonal polynomials: even for cases where we have explicit formulae (e.g. Chebyshev polynomials $T_n(x) = \cos n \arccos x$), using the recurrence avoids evaluating trigonometric functions. The following shows, surprisingly, that evaluating Chebyshev polynomials using the three-term recurrence is much faster than using the explicit formula:

`using LinearAlgebra, Plots, ApproxFun, BandedMatrices`

```
function recurrence_Chebyshev(n,x)
    T = zeros(n)
    T[1] = 1.0
    T[2] = x*T[1]
    for k = 2:n-1
        T[k+1] = 2x*T[k] - T[k-1]
    end
    T
end

trig_Chebyshev(n,x) = [cos(k*acos(x)) for k=0:n-1]

n = 10
@show norm(recurrence_Chebyshev(n, 0.1) - trig_Chebyshev(n,0.1),Inf)

n = 1_000_000
@time recurrence_Chebyshev(n, 0.1)
@time trig_Chebyshev(n,0.1);

norm(recurrence_Chebyshev(n, 0.1) - trig_Chebyshev(n, 0.1), Inf) = 1.110223
0246251565e-16
0.004717 seconds (2 allocations: 7.629 MiB)
0.029896 seconds (2 allocations: 7.629 MiB)
```

Theorem (three-term recurrence) Suppose $\{p_n(x)\}$ are a family of orthogonal polynomials w.r.t. a weight $w(x)$. Then there exists constants a_n , $b_n \neq 0$ and $c_n \neq 0$ such that

$$\begin{aligned} xp_0(x) &= a_0p_0(x) + b_0p_1(x) \\ xp_n(x) &= c_np_{n-1}(x) + a_np_n(x) + b_np_{n+1}(x) \end{aligned}$$

Proof The first part follows since $p_0(x)$ and $p_1(x)$ span all degree 1 polynomials.

The second part follows essentially because multiplication by x is "self-adjoint", that is,

$$\langle xf, g \rangle = \int_a^b xf(x)g(x)w(x)dx = \langle f, xg \rangle$$

Therefore, if f_m is a degree $m < n - 1$ polynomial, we have

$$\langle xp_n, f_m \rangle = \langle p_n, xf_m \rangle = 0.$$

In particular, if we write

$$xp_n(x) = \sum_{k=0}^{n+1} C_k p_k(x)$$

then

$$C_k = \frac{\langle xp_n, p_k \rangle}{\|p_k\|^2} = 0$$

if $k < n - 1$.

Note that

$$C_{n+1} = b_n = \frac{\langle p_{n+1}, xp_n \rangle}{\|p_{n+1}\|^2} \neq 0$$

since $xp_n = k_n x^{n+1} + O(x^n)$ is precisely degree n . Further,

$$C_{n-1} = c_{n-1} = \frac{\langle p_{n-1}, xp_n \rangle}{\|p_{n-1}\|^2} = \frac{\langle p_n, xp_{n-1} \rangle}{\|p_{n-1}\|^2} = b_{n-1} \frac{\|p_n\|^2}{\|p_{n-1}\|^2} \neq 0.$$

■

Clearly if p_n is monic then so is xp_n which leads to the following:

Corollary (monic 3-term recurrence) If $\{p_n\}$ are monic then $b_n = 1$.

1.3.2 Jacobi matrices and multiplication by x

The three-term recurrence can also be interpreted as an infinite tridiagonal matrix known as the Jacobi matrix:

Corollary (Jacobi matrix) For

$$P(x) := [p_0(x)|p_1(x)|\cdots]$$

we have

$$xP(x) = P(x) \underbrace{\begin{bmatrix} a_0 & c_0 & & \\ b_0 & a_1 & c_1 & \\ & b_1 & a_2 & \ddots \\ & & \ddots & \ddots \end{bmatrix}}_X$$

Here is the Jacobi matrix for the Chebyshev polynomials:

$X = \text{Multiplication}(\text{Fun}(x \rightarrow x), \text{Chebyshev}())$

ConcreteMultiplication : Chebyshev() \rightarrow Chebyshev()

```

0.0  0.5  .   .   .   .   .   .   .   .   .   .
1.0  0.0  0.5  .   .   .   .   .   .   .   .   .
.   0.5  0.0  0.5  .   .   .   .   .   .   .   .
.   .   0.5  0.0  0.5  .   .   .   .   .   .   .
.   .   .   0.5  0.0  0.5  .   .   .   .   .   .
.   .   .   .   0.5  0.0  0.5  .   .   .   .   .
.   .   .   .   .   0.5  0.0  0.5  .   .   .   .
.   .   .   .   .   .   0.5  0.0  0.5  .   .   .
.   .   .   .   .   .   .   0.5  0.0  0.5  .   .
.   .   .   .   .   .   .   .   0.5  0.0  .   .
.   .   .   .   .   .   .   .   .   .   .   .

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For the special cases of orthonormal polynomials we have extra structure:

Corollary (orthonormal 3-term recurrence) If $\{q_n\}$ are orthonormal then its recurrence coefficients satisfy $c_n = b_n$. That is, the Jacobi matrix is symmetric:

$$X = \begin{bmatrix} a_0 & b_0 & & \\ b_0 & a_1 & b_1 & \\ & b_1 & a_2 & \ddots \\ & & \ddots & \ddots \end{bmatrix}$$

Proof

$$b_n = \langle xq_n, q_{n+1} \rangle = \langle q_n, xq_{n+1} \rangle = c_n.$$

■