Applied Complex Analysis (2021)

1 Lecture 18: Orthogonal polynomials

We now introduce orthogonal polynomials (OPs). These are **fundamental** for computational mathematics, with applications in

1. Function approximation
2. Quadrature (calculating integrals)
3. Solving differential equations
4. Spectral analysis of Schrödinger operators

We will investigate the properties of *general* OPs, in this lecture:

1. Definition of orthogonal polynomials
2. Three-term recurrence relationships
3. Function approximation with orthogonal polynomials
4. Construction of orthogonal polynomials via Gram–Schmidt process

1.1 Definition of orthogonal polynomials

Let $p_0(x), p_1(x), p_2(x), \ldots$ be a sequence of polynomials such that $p_n(x)$ is exactly of degree n, that is,

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

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

$$\langle f, g \rangle := \int_a^b f(x)g(x)w(x)\mathrm{d}x$$

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

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

Because w is continuous, we have

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

Orthogonal polymomials 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 I) 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 $k \leq n-1$

$$\langle p_k, p_k \rangle c_k = \langle p_n - r_n, p_k \rangle = \langle p_n, p_k \rangle - \langle r_n, p_k \rangle = 0 - 0 = 0$$

which shows all c_k are zero.

■

Corollary (Uniqueness of OPs I) 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.

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 it's not unique: we can multiply by ± 1 without changing the norm.

Remark The classical OPs are neither monic nor orthonormal (apart from one case). Many people make the mistake of using orthonormal polynomials for computations. But there is a good reason to use classical OPs: their properties result in rational formulae, whereas orthonormal polynomials require square roots. This makes a performance difference.

1.2 Function approximation with orthogonal polynomials

A basic usage of orthogonal polynomials is for polynomial approximation. Suppose $f(x)$ is a degree $n-1$ polynomial. Since $\{p_0(x), \ldots, p_{n-1}(x)\}$ span all degree $n-1$ polynomials, we know that

$$f(x) = \sum_{k=0}^{n-1} f_k p_k(x)$$

where

$$f_k = \frac{\langle f, p_k \rangle}{\langle p_k, p_k \rangle}$$

Sometimes, we want to incorporate the weight into the approximation. This is typically one of two forms, depending on the application:

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

or

$$f(x) = \sqrt{w(x)} \sum_{k=0}^{\infty} f_k p_k(x)$$

The $w(x)p_k(x)$ or $\sqrt{w(x)}p_k(x)$ are called weighted polynomials.

1.3 Jacobi operators and three-term recurrences for general orthogonal polynomials

1.3.1 Three-term recurrence relationships

A central theme: if you know the Jacobi operator / 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 $T_n(x) = \cos n \mathrm{acos}\, x$), usigng the recurrence avoids evaluating trigonometric functions.

Every family of orthogonal polynomials has a three-term recurrence relationship:

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 $a_n \neq 0$, b_n and c_n such that

$$\begin{aligned} xp_0(x) &= a_0 p_0(x) + b_0 p_1(x) \\ xp_n(x) &= c_n p_{n-1}(x) + a_n p_n(x) + b_n p_{n+1}(x) \end{aligned}$$

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,

$$\langle xf, g\rangle = \int_a^b xf(x)g(x)w(x)\mathrm{d}x = \langle f, xg\rangle$$

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 $k < n-1$.

■

Monic polynomials clearly have $b_n = 1$. Orthonormal polynomials have an even simpler form:

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

$$xq_0(x) = a_0 q_0(x) + b_0 q_1(x)$$
$$xq_n(x) = b_{n-1} q_{n-1}(x) + a_n q_n(x) + b_n q_{n+1}(x)$$

Proof Follows again by self-adjointness of multiplication by x:

$$c_n = \langle x q_n, q_{n-1} \rangle = \langle q_n, x q_{n-1} \rangle = \langle x q_{n-1}, q_n \rangle = b_{n-1}$$

■

Corollary (symmetric three-term recurrence implies orthonormality) Suppose $\{p_n(x)\}$ are a family of orthogonal polynomials w.r.t. a weight $w(x)$ such that

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

with $b_n \neq 0$. Suppose further that $\|p_0\| = 1$. Then p_n must be orthonormal.

Proof This follows from

$$b_n = \frac{\langle xp_n, p_{n+1}\rangle}{\|p_{n+1}\|^2} = \frac{\langle xp_{n+1}, p_n\rangle}{\|p_{n+1}\|^2} = b_n\frac{\|p_n\|^2}{\|p_{n+1}\|^2}$$

which implies

$$\|p_{n+1}\|^2 = \|p_n\|^2 = \cdots = \|p_0\|^2 = 1$$

■ **Remark** We can scale $w(x)$ by a constant without changing the orthogonality properties, hence we can make $\|p_0\| = 1$ by changing the weight.

Remark This is beyond the scope of this course, but satisfying a three-term recurrence like this such that coefficients are bounded with $p_0(x) = 1$ is sufficient to show that there exists a $w(x)$ (or more accurately, a Borel measure) such that $p_n(x)$ are orthogonal w.r.t. w. The relationship between the coefficients a_n, b_n and the $w(x)$ is an object of study in spectral theory, particularly when the coefficients are periodic, quasi-periodic or random.

1.4 Jacobi operators and multiplication by x

We can rewrite the three-term recurrence as

$$x \begin{pmatrix} p_0(x) \\ p_1(x) \\ p_2(x) \\ \vdots \end{pmatrix} = J \begin{pmatrix} p_0(x) \\ p_1(x) \\ p_2(x) \\ \vdots \end{pmatrix}$$

where J is a Jacobi operator, an infinite-dimensional tridiagonal matrix:

$$J = \begin{pmatrix} a_0 & b_0 & & & \\ c_1 & a_1 & b_1 & & \\ & c_2 & a_2 & b_2 & \\ & & c_3 & a_3 & \ddots \\ & & & \ddots & \ddots \end{pmatrix}$$

When the polynomials are monic, we have 1 on the superdiagonal. When we have an orthonormal basis, then J is symmetric:

$$J = \begin{pmatrix} a_0 & b_0 & & & \\ b_0 & a_1 & b_1 & & \\ & b_1 & a_2 & b_2 & \\ & & b_2 & a_3 & \ddots \\ & & & \ddots & \ddots \end{pmatrix}$$

Given a polynomial expansion, J tells us how to multiply by x in coefficient space, that is, if

$$f(x) = \sum_{k=0}^{\infty} f_k p_k(x) = (p_0(x), p_1(x), \ldots) \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \end{pmatrix}$$

then (provided the relevant sums converge absolutely and uniformly)

$$xf(x) = x(p_0(x), p_1(x), \ldots) \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \end{pmatrix} = \left(J \begin{pmatrix} p_0(x) \\ p_1(x) \\ p_2(x) \\ \vdots \end{pmatrix} \right)^{\top} \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \end{pmatrix} = (p_0(x), p_1(x), \ldots) X \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \end{pmatrix}$$

where $X := J^{\top}$.

1.4.1 Evaluating polynomials

We can use the three-term recurrence to construct the polynomials. One way to express this is in the language of linear algebra. Suppose we are given $p_0(x) = k_0$ (where $k_0 = 1$ is pretty much always the case in practice). This can be written in matrix form as

$$(1, 0, 0, 0, 0, \ldots) \begin{pmatrix} p_0(x) \\ p_1(x) \\ p_2(x) \\ \vdots \end{pmatrix} = k_0$$

We can combine this with the Jacobi operator to get

$$\underbrace{\begin{pmatrix} 1 & & & & & \\ a_0 - x & b_0 & & & & \\ c_1 & a_1 - x & b_1 & & & \\ & c_2 & a_2 - x & b_2 & & \\ & & c_3 & a_3 - x & b_3 & \\ & & & \ddots & \ddots & \ddots \end{pmatrix}}_{L_x} \begin{pmatrix} p_0(x) \\ p_1(x) \\ p_2(x) \\ \vdots \end{pmatrix} = \begin{pmatrix} k_0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}$$

For x fixed, this is a lower triangular system, that is, the polynomials equal

$$k_0 L_x^{-1} \mathbf{e}_0$$

This can be solved via forward recurrence:

$$
\begin{aligned}
p_0(x) &= k_0 \\
p_1(x) &= \frac{(x-a_0)p_0(x)}{b_0} \\
p_2(x) &= \frac{(x-a_1)p_0(x) - c_1 p_0(x)}{b_1} \\
p_3(x) &= \frac{(x-a_2)p_1(x) - c_2 p_1(x)}{b_2} \\
&\vdots
\end{aligned}
$$

We can use this to evaluate functions as well:

$$
f(x) = (p_0(x), p_1(x), \ldots) \begin{pmatrix} f_0 \\ f_1 \\ \vdots \end{pmatrix} = k_0 \mathbf{e}_0^\top L_x^{-\top} \begin{pmatrix} f_0 \\ f_1 \\ \vdots \end{pmatrix}
$$

when f is a degree $n-1$ polynomial, this becomes a problem of inverting an upper triangular matrix, that is, we want to solve the $n \times n$ system

$$\underbrace{\begin{pmatrix} 1 & a_0 - x & c_1 & & & \\ & b_0 & a_1 - x & c_2 & & \\ & & b_1 & a_2 - x & \ddots & \\ & & & b_2 & \ddots & c_{n-2} \\ & & & & \ddots & a_{n-2} - x \\ & & & & & b_{n-2} \end{pmatrix}}_{L_x^\top} \begin{pmatrix} \gamma_0 \\ \vdots \\ \gamma_{n-1} \end{pmatrix}$$

so that $f(x)/k_0 = \gamma_0$. We we can solve this via back-substitution:

$$\begin{aligned} \gamma_{n-1} &= \frac{f_{n-1}}{b_{n-2}} \\ \gamma_{n-2} &= \frac{f_{n-2} - (a_{n-2} - x)\gamma_{n-1}}{b_{n-3}} \\ \gamma_{n-3} &= \frac{f_{n-3} - (a_{n-3} - x)\gamma_{n-2} - c_{n-2}\gamma_{n-1}}{b_{n-4}} \\ &\vdots \\ \gamma_1 &= \frac{f_1 - (a_1 - x)\gamma_2 - c_2\gamma_3}{b_0} \\ \gamma_0 &= f_0 - (a_0 - x)\gamma_1 - c_1\gamma_2 \end{aligned}$$

We give examples of these algorithms applied to Chebyshev polynomials in the next lecture.

1.5 Gram–Schmidt algorithm

In general we don't have nice formulae for OPs but we can always construct them via the Gram–Schmidt process:

Proposition (Gram–Schmidt) Define

$$\begin{aligned} p_0(x) &= 1 \\ q_0(x) &= \frac{1}{\|p_0\|} \\ p_{n+1}(x) &= x q_n(x) - \sum_{k=0}^{n} \langle x q_n, q_k \rangle \, q_k(x) \\ q_{n+1}(x) &= \frac{p_{n+1}(x)}{\|p_{n+1}\|} \end{aligned}$$

Then $q_0(x), q_1(x), \ldots$ are orthonormal w.r.t. w.

Proof By linearity we have

$$\langle p_{n+1}, q_j \rangle = \left\langle x q_n - \sum_{k=0}^{n} \langle x q_n, q_k \rangle q_k, q_j \right\rangle = \langle x q_n, q_j \rangle - \langle x q_n, q_j \rangle \, \langle q_j, q_j \rangle = 0$$

Thus p_{n+1} is orthogonal to all lower degree polynomials. So is q_{n+1}, since it is a constant multiple of p_{n+1}.

■

Let's make our own family of OPs:

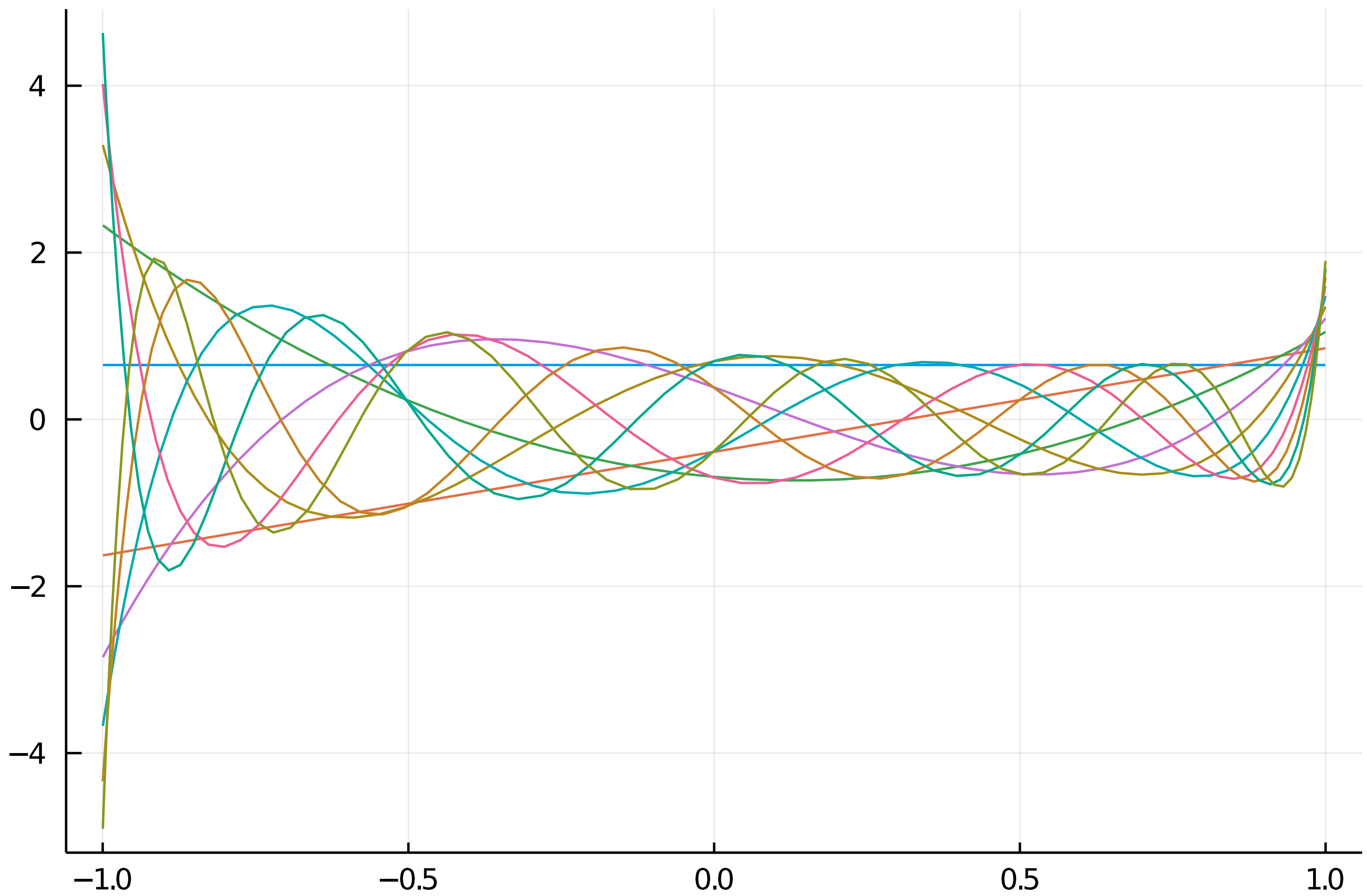
```
using ApproxFun, Plots
x = Fun()
w = exp(x)
ip = (f,g) -> sum(f*g*w)
nrm = f     -> sqrt(ip(f,f))
n = 10
q = Array{Fun}(undef,n)
p = Array{Fun}(undef,n)
p[1] = Fun(1, -1 .. 1 )
q[1] = p[1]/nrm(p[1])
for k=1:n-1
    p[k+1] = x*q[k]
    for j=1:k
        p[k+1] -= ip(p[k+1],q[j])*q[j]
    end
    q[k+1] = p[k+1]/nrm(p[k+1])
end

@show sum(q[2]*q[4]*w)

p = plot(; legend=false)
for k=1:10
```

```
    plot!(q[k])
end
p
```

sum(q[2] * q[4] * w) = 8.167294965333305e-16



The three-term recurrence means we can simplify Gram–Schmidt, and calculate the recurrence coefficients at the same time:

Proposition (Gram–Schmidt) Define

$$
\begin{aligned}
p_0(x) &= 1 \\
q_0(x) &= \frac{1}{\|p_0\|} \\
a_n &= \langle x q_n, q_n \rangle \\
b_{n-1} &= \langle x q_n, q_{n-1} \rangle \\
p_{n+1}(x) &= x q_n(x) - a_n q_n(x) - b_{n-1} q_{n-1}(x) \\
q_{n+1}(x) &= \frac{p_{n+1}(x)}{\|p_{n+1}\|}
\end{aligned}
$$

Then $q_0(x), q_1(x), \ldots$ are orthonormal w.r.t. w.

Remark This can be made a bit more efficient by using $\|p_{n+1}\|$ to calculate b_n.

```
x = Fun()
w = exp(x)
ip = (f,g) -> sum(f*g*w)
nrm = f     -> sqrt(ip(f,f))
n = 10
q = Array{Fun}(undef, n)
p = Array{Fun}(undef, n)
```

```julia
a = zeros(n)
b = zeros(n)
p[1] = Fun(1, -1 .. 1 )
q[1] = p[1]/nrm(p[1])

p[2] = x*q[1]
a[1] = ip(p[2],q[1])
p[2] -= a[1]*q[1]
q[2] = p[2]/nrm(p[2])

for k=2:n-1
    p[k+1] = x*q[k]
    b[k-1] =ip(p[k+1],q[k-1])
    a[k] = ip(p[k+1],q[k])
    p[k+1] = p[k+1] - a[k]q[k] - b[k-1]q[k-1]
    q[k+1] = p[k+1]/nrm(p[k+1])
end

ip(q[5],q[2]) # shows orthogonality (to numerical accuracy)
```

```
1.0755285551056204e-15
```

Here we see a plot of the first 10 polynomials:

```julia
p = plot(; legend=false)
```

```julia
for k=1:10
    plot!(q[k])
end
p
```