MATH50003 Numerical Analysis

VI.1 Orthogonal Polynomials

Dr Sheehan Olver

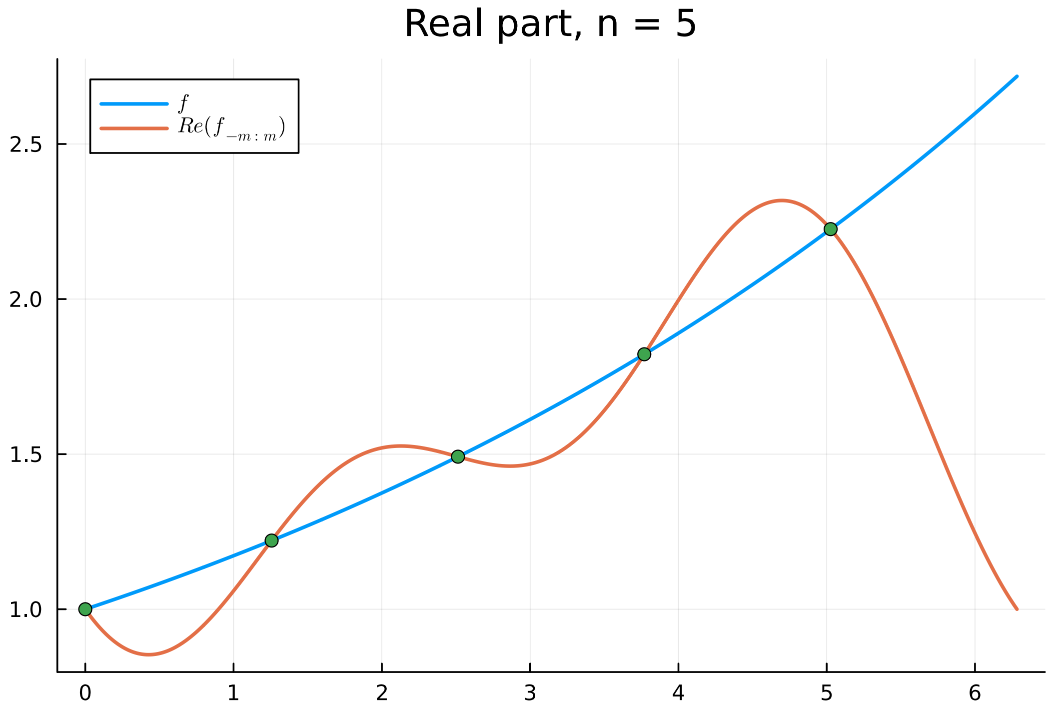
Part VI

Orthogonal Polynomials

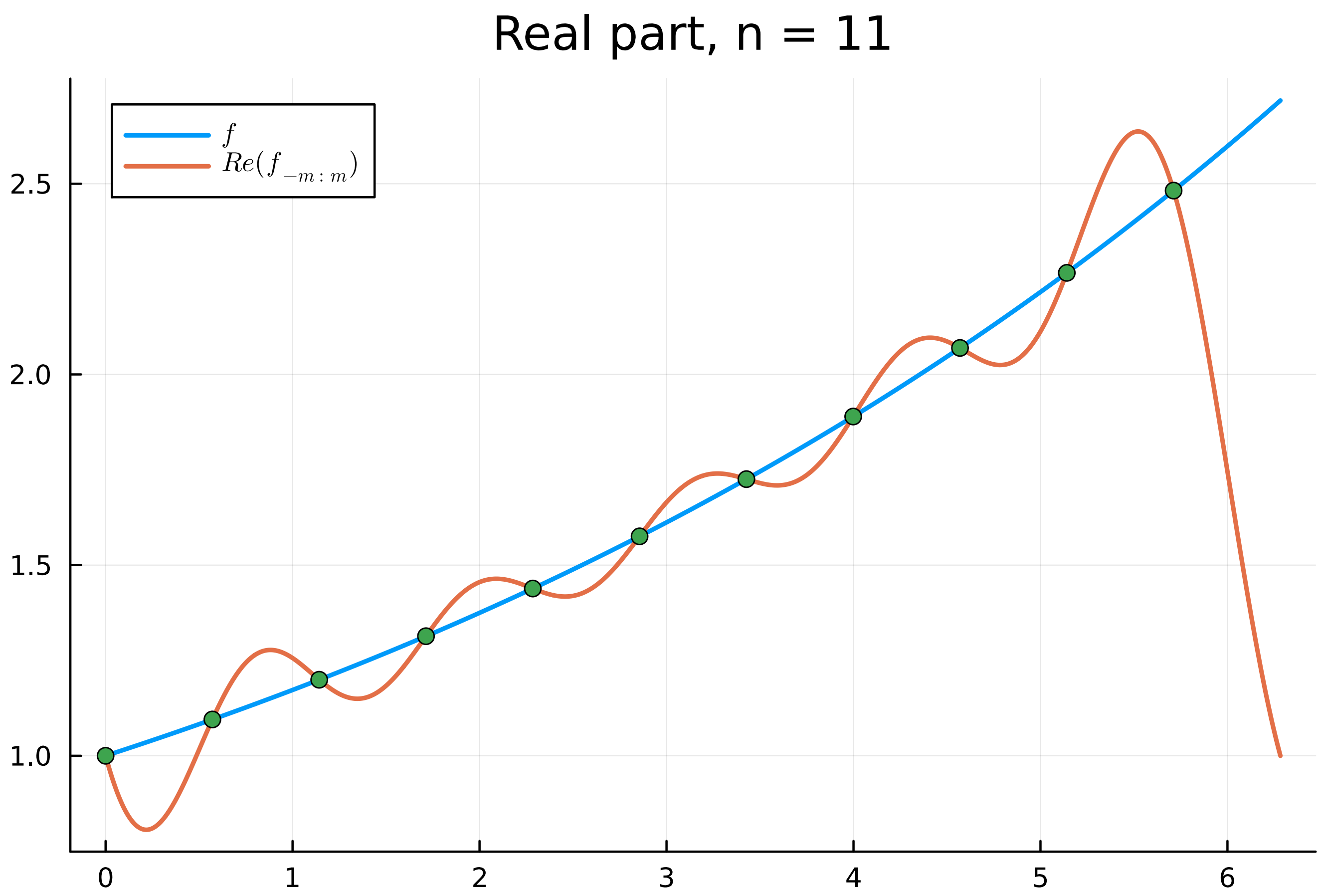
1. General Orthogonal Polynomials and basic properties
2. Classical Orthogonal Polynomials with special structure
3. Gaussian Quadrature for high-accuracy integration

What’s wrong with Fourier?

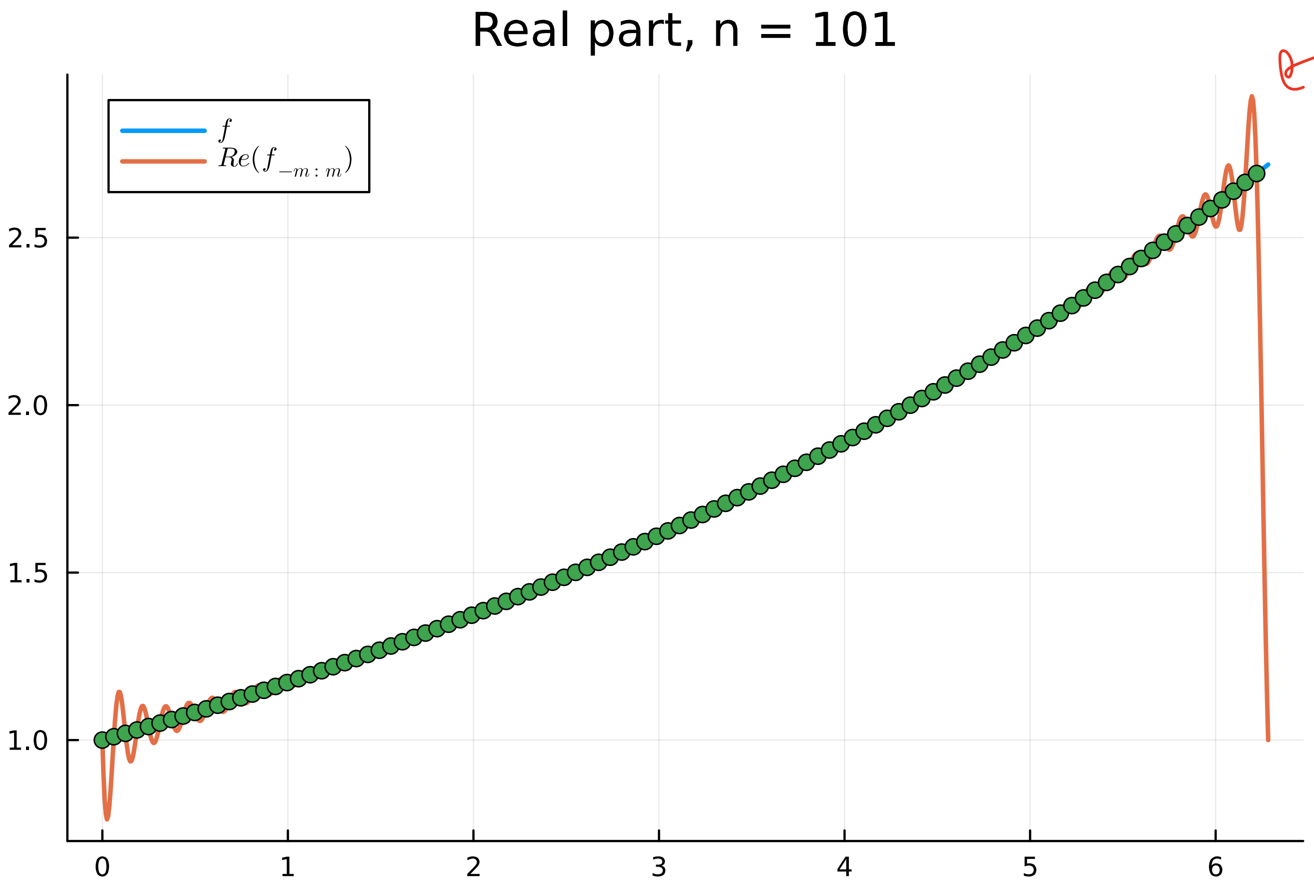
Doesn’t converge uniformly if a function isn’t periodic



e^{θ}



Real part, n = 11
f
$Re(f_{-m:m})$
2.5
2.0
1.5
1.0
0
1
2
3
4
5
6

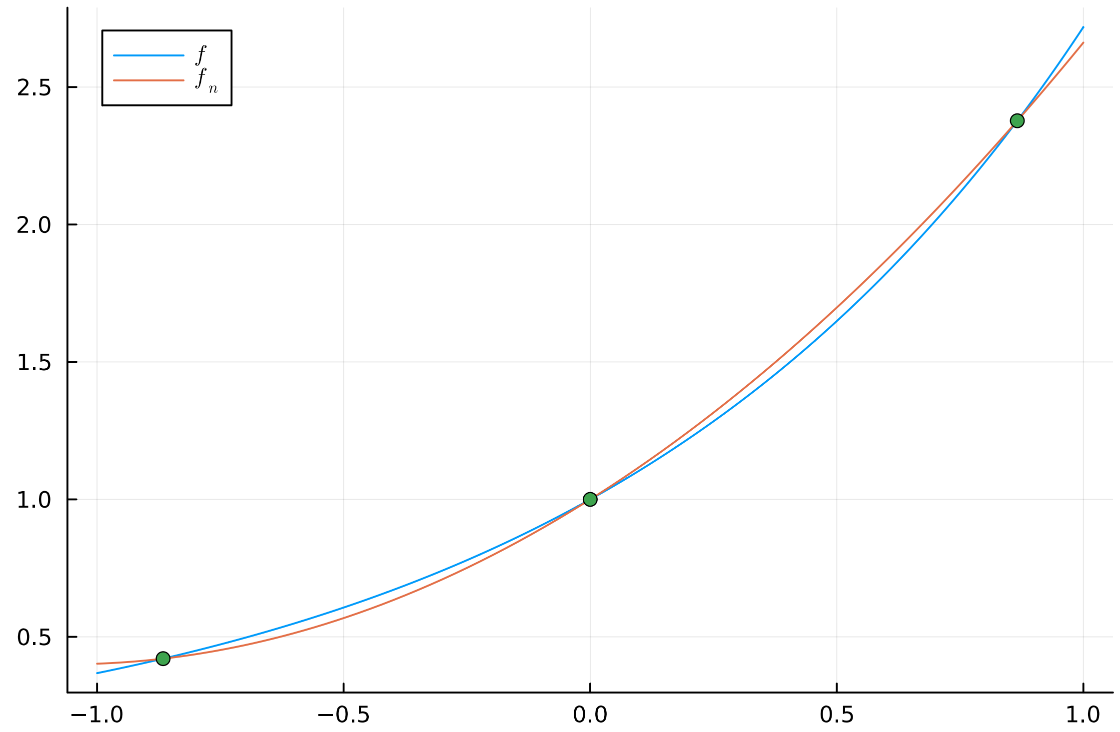


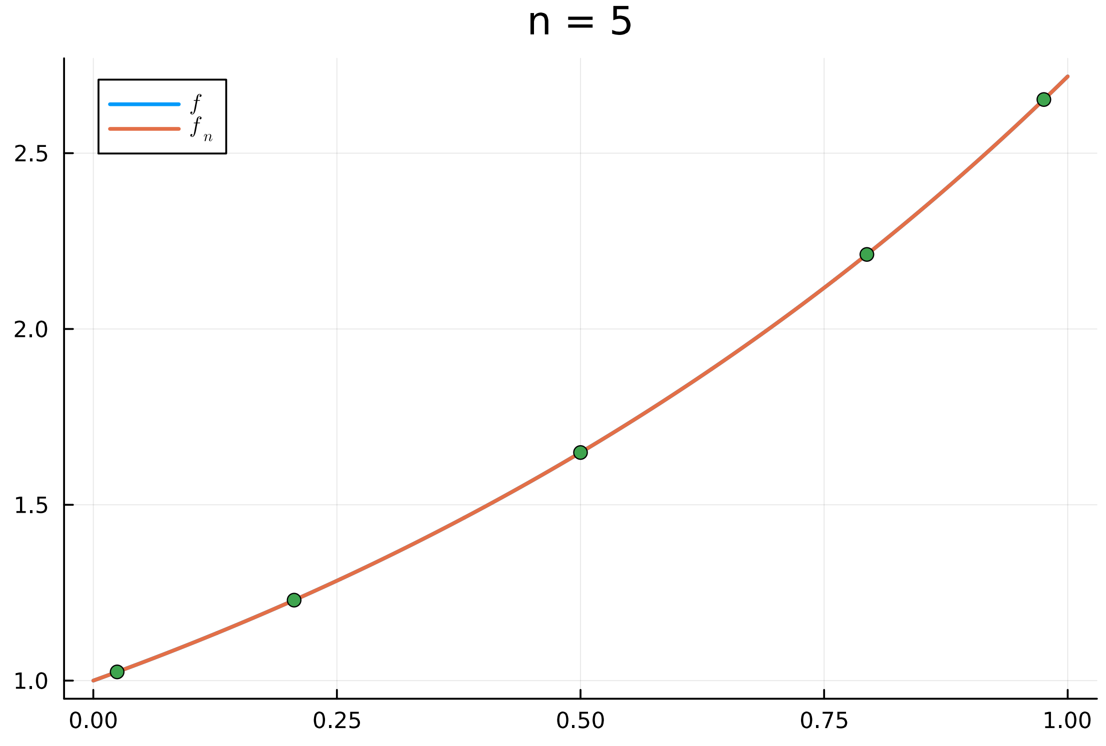
Gibb's phenomenon?

non-uniform convergence

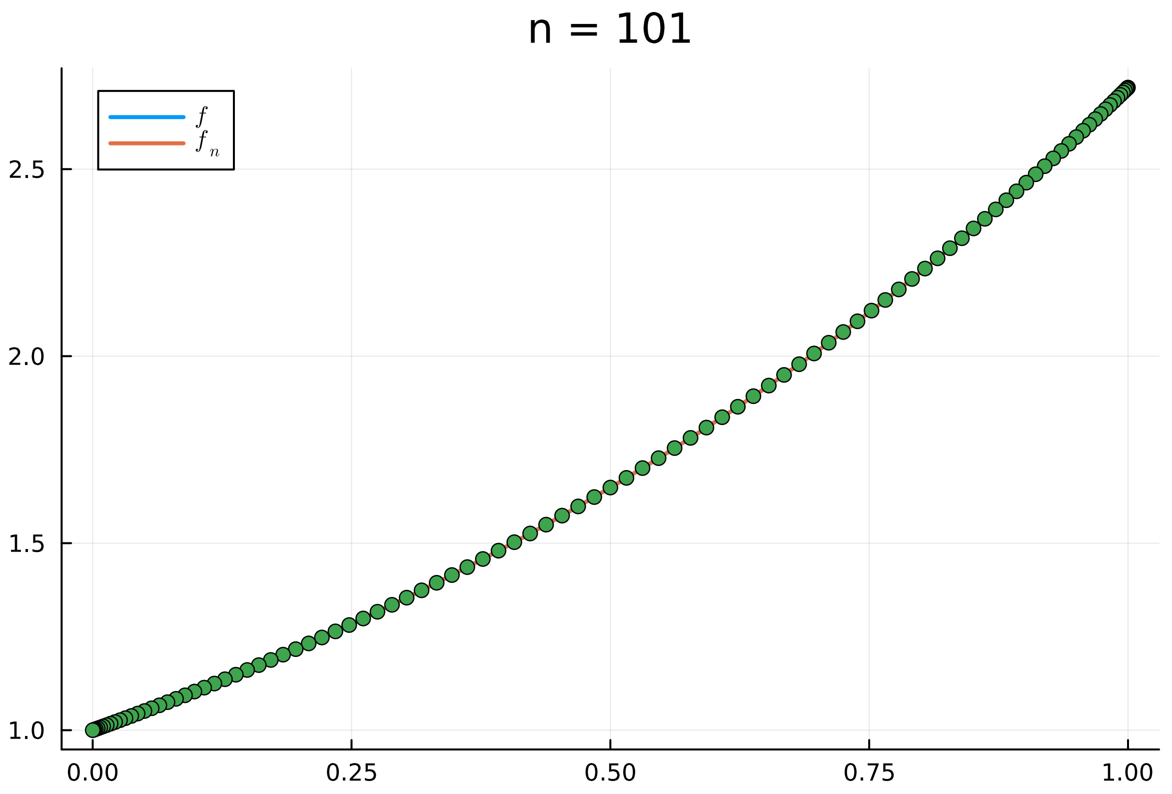
Instead use orthogonal polynomials w/ special points

We already saw monomials aren't reliable for interpolation





n = 5
f
f_n
2.5
2.0
1.5
1.0
0.00
0.25
0.50
0.75
1.00



n = 101
f
f_n
2.5
2.0
1.5
1.0
0.00
0.25
0.50
0.75
1.00

VI.1.1 General properties

Definition of Orthogonal Polynomials and basic properties

Definition 35 (graded polynomial basis)**.** A set of polynomials $\{p_0(x), p_1(x), \ldots\}$ is *graded* if p_n is precisely degree n: i.e.,

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

for $k_n \neq 0$.

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

We want to construct

$$p_0(x) = k_0$$

$$p_1(x) = k_1 x + O(1)$$

$$p_2(x) = k_2 x^2 + O(x)$$

$$\vdots$$

orthogonal wrt inner product. Any graded polynomials are a basis of polynomials.

Definition 36 (Orthogonal Polynomials)**.** Given an (integrable) *weight* $w(x) > 0$ for $x \in (a, b)$, which defines a continuous inner product

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

a graded polynomial basis $\{p_0(x), p_1(x), \ldots\}$ are *orthogonal polynomials (OPs)* if

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

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

Examples:

$w(x) = 1$ on $[0,1]$

$= \sqrt{1-x^2}$ on $[-1,1]$

$= e^{-x^2}$ on $(-\infty, \infty)$

Definition 37 (Orthonormal Polynomials)**.** A set of orthogonal polynomials $\{q_0(x), q_1(x), \ldots\}$ are *orthonormal* if $\|q_n\| = 1$.

Definition 38 (Monic Orthogonal Polynomials)**.** A set of orthogonal polynomials $\{\pi_0(x), \pi_1(x), \ldots\}$ are *monic* if $k_n = 1$. I.e. $p_n(x) = x^n + O(x^{n-1})$

Proposition 13 (existence)**.** *Given a weight $w(x)$, monic orthogonal polynomials exist.*

Proof Gram-Schmidt. We know $\pi_0(x) = 1$,

Assume we know π_0 — $\pi_n(x)$.

Consider

$$\pi_{n+1}(x) = \underbrace{x\pi_n(x)}_{= x^{n+1} + O(x^n)} - \frac{\langle x\pi_n, \pi_n\rangle}{\|\pi_n\|^2}\pi_n(x)$$

$$- \frac{\langle x\pi_n, \pi_{n-1}\rangle}{\|\pi_{n-1}\|^2}\pi_{n-1}(x)$$

$$- \cdots - \langle x\pi_n, \pi_0\rangle\, \pi_0(x)$$

$$\overline{\qquad\qquad\qquad}$$
$$\|\pi_0\|^2$$

so that

$$\langle \pi_{n+1}, \pi_m \rangle = \langle x\pi_n, \pi_m \rangle - \frac{\langle x\pi_n, \pi_m \rangle}{\|\pi_m\|^2} \langle \pi_m, \pi_m \rangle$$

$$= 0 .$$

Proposition 14 (expansion)**.** *If $r(x)$ is a degree n polynomial and $\{p_n\}$ are orthogonal then*

$$r(x) = \sum_{k=0}^{n} \frac{\langle p_k, r\rangle}{\|p_k\|^2} p_k(x).$$

Note for $\{q_n\}$ orthonormal we have

$$r(x) = \sum_{k=0}^{n} \langle q_k, r\rangle q_k(x).$$

since $\|q_n\| = 1$.

Proof

$\{p_n\}$ is a basis $\Rightarrow$ $\exists\, r_k \in \mathbb{R}$ s.t.

$$r(x) = \sum_{k=0}^{n} r_k\, p_k(x)$$

But

$$\langle r, p_j\rangle = \sum_{k=0}^{n} r_k \underbrace{\langle p_k, p_j\rangle} = r_j \|p_j\|^2$$

$= 0$ if $k \neq j$

Corollary 5 (zero inner product). *If a degree n polynomial r satisfies*

$$0 = \langle p_0, r \rangle = \ldots = \langle p_n, r \rangle$$

then $r = 0$.

Corollary 6 (uniqueness)**.** *Monic orthogonal polynomials are unique.*

<u>Proof</u> Suppose $p_n(x) = x^n + O(x^{n-1})$ are also monic OPs.

Consider

$$r(x) = \overbrace{p_n(x)}^{x^n + O(x^{n-1})} - \overbrace{\pi_n(x)}^{x^n + O(x^{n-1})} = O(x^{n-1})$$

constructed via Gram Schmidt

But for $k = 0, \ldots, n-1$

$$\langle r, \pi_k \rangle = \langle p_n, \pi_k \rangle = \sum_{j=0}^{k} c_k \langle p_n, p_j \rangle = 0,$$

$\sum_{j=0}^{k} c_j p_j(x)$ $= 0$ since $j < n$

Theorem 14 (orthogonal to lower degree). *Given a weight $w(x)$, a polynomial*

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

with $k_n \neq 0$ satisfies

$$\langle p, f_m \rangle = 0$$

for all polynomials f_m of degree $m < n$ if and only if $p(x) = k_n \pi_n(x)$ where $\pi_n(x)$ are the monic orthogonal polynomials. Therefore an orthogonal polynomial is uniquely defined by the weight and leading order coefficient k_n.

Proof PS 9.

Implication: $w(x)$ and k_n uniquely define $p_n(x)$. Ie, if we show orthogonality & and deduce k_n we prove $= p_n(x)$.

VI.1.2 Three-term recurrence

OPs satisfy a simple relationship between consecutive polynomails

Theorem 15 (3-term recurrence, 2nd form)**.** *If* $\{p_n\}$ *are OPs then there exist real constants* $a_n b_n, c_{n-1}$ *such that*

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

where $b_n \neq 0$ *and* $c_{n-1} \neq 0$.

Compare w/ Taylor series $p_n(z) = z^n$ where

$$z p_n(z) = p_{n+1}(z)$$

Proof Since $p_n(x)$ are a basis:

$$x p_n(x) = b_n p_{n+1}(x) + a_n p_n(x) + c_{n-1} p_{n-1}(x)$$

degree $n+1$

$$+ \sum_{j=0}^{n-2} \alpha_j p_j(x)$$

degree $j+1 \leq n-1 < n$

But

$$\alpha_j = \frac{\langle x p_n, p_j \rangle}{\|p_j\|^2} = \frac{\langle p_n, x p_j \rangle}{\|p_j\|^2} \underset{\text{Thm 14}}{=} 0$$

Need to show $b_n, c_n \neq 0$. $b_n \neq 0$ is immediate. But

$$c_{n-1} = \frac{\langle x p_n, p_{n-1} \rangle}{\|p_{n-1}\|^2} = \frac{\langle p_n, x p_{n-1} \rangle}{\|p_{n-1}\|^2}$$

$$= \underbrace{b_{n-1}}_{\langle x p_{n-1}, p_n \rangle / \|p_n\|^2} \frac{\|p_n\|^2}{\|p_{n-1}\|^2} \neq 0$$

Corollary 7 (monic 3-term recurrence)**.** *$\{\pi_n\}$ are monic if and only if $b_n = 1$.*

MEQs: Please fill out.

Positive feedback (what worked well, etc.) also helpful to know where to focus improvement

We can use 3-term recurrence to simplify Gram-Schmidt (Stieltjes)

Example 23 (constructing monic OPs).

$w(x) = 1$ on $[0,1]$, ie wrt

$$\langle f, g \rangle := \int_0^1 f(x) g(x) \, dx.$$

$\pi_0(x) = 1$ so that $\|\pi_0\|^2 = \int_0^1 dx = 1$.

We know

$$x \pi_0(x) = \underbrace{a_0}_{\text{unkown}} \pi_0(x) + \underbrace{\pi_1(x)}_{\text{unkown}}$$

Where

$$\underbrace{\langle x\pi_0, \pi_0 \rangle} = a_0 \underbrace{\langle \pi_0, \pi_0 \rangle} + \underbrace{\langle \pi_1, \pi_0 \rangle}$$

$\int_0^1 x\,dx = 1/2$ $\qquad = 1 \qquad = 0$

$\Rightarrow \quad a_0 = 1/2 \quad \Rightarrow$

$\pi_1(x) = x\pi_0(x) - a_0\pi_0(x) = x - 1/2$

where $\quad \|\pi_1\|^2 = \int_0^1 (x - 1/2)^2 dx = \frac{1}{12}$

Then

$$\overbrace{x\pi_1(x)}^{= x^2 + O(x)} = c_0\pi_0(x) + a_1\pi_1(x) + \overbrace{\pi_2(x)}^{x^2 + O(x)}$$

where

$$\underbrace{\langle x\pi_1, \pi_0\rangle}_{} = c_0 \cancel{\|\pi_0\|^2}$$

$\int_0^1 x(x - 1/2)\,dx = 1/12 \Rightarrow \quad c_0 = 1/12, \quad$ Also

$$\langle x\pi_1, \pi_1\rangle = a_1 \|\pi_1\|^2 = 12\int_0^1 x\left(x-\tfrac{1}{2}\right)^2 dx = \tfrac{1}{2}.$$

$$\Rightarrow \quad \pi_2(x) = x\pi_1(x) - \frac{1}{12}\pi_0(x) - \frac{1}{2}\pi_1(x)$$

$$= x\left(x-\tfrac{1}{2}\right) - \frac{1}{12} - \frac{\left(x-\tfrac{1}{2}\right)}{2} = x^2 - x + \tfrac{1}{6}.$$

Then

No $\pi_0(x)$ term

$$x\pi_2(x) = c_1\pi_1(x) + a_2\pi_2(x) + \pi_3(x)$$

where

$$c_1 = \frac{\langle x\pi_2, \pi_1\rangle}{\|\pi_1\|^2} = \tfrac{1}{15}$$

$$a_2 = \frac{\langle x\pi_2, \pi_2\rangle}{\|\pi_2\|^2} = \tfrac{1}{2} \Rightarrow$$

$$\pi_3(x) = x\pi_2 - \frac{\pi_1}{15} - \frac{\pi_2}{2} = x^3 - \frac{3x^2}{2} + \frac{3x}{5} - \frac{1}{20}.$$

VI.1.3 Jacobi matrices

Multiplying OPs by polynomials has a simple form

Corollary 8 (multiplication matrix). *For*

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

then we have

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

Analogous to Taylor series?

$$z\left[1 \mid z \mid z^2 \mid \text{—}\right] = \left[1 \mid z \mid z^2 \mid \text{—}\right]\begin{bmatrix} 0 & & & \\ 1 & & & \\ & 1 & & \\ & & \ddots & \end{bmatrix}$$

Proof

$$x\left[p_0 \mid p_1 \mid \text{—}\right] = \left[x p_0 \mid x p_1 \mid \text{—}\right]$$

$$= \left[a_0 p_0 + b_0 p_1 \mid c_0 p_0 + a_1 p_1 + b_1 p_2 \mid \text{—}\right]$$

$$= \left[p_0 \mid p_1 \mid \text{—}\right] X$$

Note

$$x^2 P(x) = x\, x P(x) = x P(x) X$$

$$= P(x) X^2$$

Or more generally

$a(x) = \sum_{k=0}^{n} a_k X^k$ then

$$a(x) P(x) = P(x) \underbrace{a(X)}_{\sum_{k=0}^{n} a_k X^k}$$

Corollary 9 (Jacobi matrix). *The multiplication matrix of a family of orthogonal polynomials $p_n(x)$ is symmetric,*

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

if and only if $p_n(x)$ is up-to-sign a fixed constant scaling of orthonormal: for $q_n(x) := \pi_n(x)/\|\pi_n\|$ we have for a fixed $\alpha \in \mathbb{R}$ and $s_n \in \{-1, 1\}$

$$p_n(x) = \alpha \underbrace{s_n}_{\pm 1} q_n(x).$$

Proof (ortho $\Rightarrow$ Sym Jacobi)

Suppose $p_n(x) = \alpha s_n q_n(x) \Rightarrow \|p_n\|^2 = \alpha^2 \|q_n\|^2$
$= \alpha^2$

Then $$b_n = \frac{\langle x p_n , p_{n+1} \rangle}{\|p_{n+1}\|^2} = \frac{\cancel{\alpha^2}\, s_n s_{n+1} \langle x q_n , q_{n+1} \rangle}{\cancel{\alpha^2}}$$

$$= \langle q_n , x q_{n+1} \rangle s_n s_{n+1}$$

$$= \frac{\langle p_n , x p_{n+1} \rangle}{\alpha^2} = c_n$$

(Sym $\Rightarrow$ Ortho)

Suppose $b_n = c_n$. Denote $p_n(x) = \alpha_n q_n(x)$

want to show $= \pm \alpha_0$

But

$$b_n = \frac{\langle x p_n , p_{n+1} \rangle}{\|p_{n+1}\|^2} = \frac{\alpha_n \cancel{\alpha_{n+1}}}{\alpha_{n+1}^{\cancel{2}}} \langle x q_n , q_{n+1} \rangle = \frac{\cancel{\alpha_n}}{\alpha_{n+1}} \frac{\langle p_n , x p_{n+1} \rangle}{\cancel{\alpha_n}\, \alpha_{n+1}} \frac{\alpha_n^2}{\|p_n\|^2}$$

$$= c_n \frac{\alpha_n^2}{\alpha_{n+1}^2} \Rightarrow \alpha_{n+1}^2 = \alpha_n^2 = \alpha_{n-1}^2 = \cdots = \alpha_0^2 \quad \text{W}$$

Example 24 (uniform weight orthonormal polynomials).

$$\langle f, g \rangle = \int_0^1 f(x) g(x) \, dx$$

Compute $q_0(x), \cdots q_3(x)$.

Method 1: Compute $q_n(x) = \dfrac{\pi_n(x)}{\|\pi_n\|^2}$

Method 2: Symmetrise the multip. matrix.

$$x [\pi_0 | \pi_1 | \cdots] = \begin{bmatrix} 1/2 & 1/12 & & & \\ 1 & 1/2 & 1/15 & & \\ & 1 & 1/2 & \ddots & \\ & & 1 & \ddots & \ddots \\ & & & \ddots & \ddots \end{bmatrix}$$

X

We know

$$q_n(x) = \underbrace{k_n}_{\text{unknown}} x^n + O(x^{n-1}) = k_n \pi_n(x)$$

$$\Rightarrow$$

$$x[q_0 | q_1 | \cdots] = x[\pi_0 | \pi_1 | \cdots] \underbrace{\begin{bmatrix} \overset{=1}{k_0} & & & \\ & k_1 & & \\ & & k_2 & \\ & & & \ddots \end{bmatrix}}_{K}$$

$$= [\pi_0 | \pi_1 | \cdots] \, X K$$

$$= [q_0 | q_1 | \cdots] \underbrace{K^{-1} X K}_{J}$$

J must be sym.

Where

$$J = \begin{bmatrix} 1 & & & \\ & k_1^{-1} & & \\ & & k_2^{-1} & \\ & & & \ddots \end{bmatrix} \begin{bmatrix} a_0 & c_0 & & & \\ 1 & a_1 & c_1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & & \ddots \end{bmatrix} \begin{bmatrix} 1 & & & \\ & k_1 & & \\ & & k_2 & \\ & & & \ddots \end{bmatrix}$$

$$= \begin{bmatrix} a_0 & c_0 k_1 & & & \\ k_1^{-1} & a_1 & c_1 \frac{k_2}{k_1} & & \\ & \frac{k_1}{k_2} & a_2 & c_2 \frac{k_3}{k_2} & \\ & & \ddots & \ddots & \ddots \end{bmatrix}$$

Symmetry implies

$$c_0 k_1 = 1/k_1 \Rightarrow k_1^2 = \frac{1}{c_0} = 12 \Rightarrow k_1 = \sqrt{12}$$

$$c_1 \frac{k_2}{k_1} = \frac{k_1}{k_2} \Rightarrow k_2^2 = \frac{k_1^2}{c_1} = 12 \cdot 15 \Rightarrow k_2 = 6\sqrt{5}$$

$$c_2 \frac{k_3}{k_2} = \frac{k_2}{k_3} \Rightarrow k_3 = 20\sqrt{7}.$$

Example 25 (expansion via Jacobi matrix).

Expand $x^3 - x + 1$ in $q_0(x), q_1(x), \ldots$

Method 1: compute inner products

Method 2: match terms

Method 3: Use Jacobi matrix. I.e.

We want to find

$$x^3 - x + 1 = c_3 q_3(x) + \cdots + c_0 q_0(x)$$

$$= \underbrace{[q_0 | q_1 | \cdots]}_{Q(x)} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \end{bmatrix}$$

We know

$q_0(x)=1$ for our inner product

$$x = x \, q_0 = x Q(x) e_0 = Q(x) \underbrace{J e_0}_{\begin{bmatrix} 1/2 \\ 1/(2\sqrt{3}) \\ 0 \\ \vdots \end{bmatrix}}$$

$$x^2 = Q(x) \underbrace{J^2 e_0}_{J(J e_0)}$$

also $x^3 = Q(x) J^3 e_0 \Rightarrow$

$$x^3 - x + 1 = Q(x)\left(J^3 \vec{e}_0 - J\vec{e}_0 + \vec{e}_0 \right)$$