Numerical Analysis Hilary Term 2021 Lecture 10: Orthogonal Polynomials

Gram-Schmidt orthogonalization procedure: the solution of the normal equations $A\alpha = \varphi$ for best least-squares polynomial approximation would be easy if A were diagonal. Instead of $\{1, x, x^2, \dots, x^n\}$ as a basis for Π_n , suppose we have a basis $\{\phi_0, \phi_1, \dots, \phi_n\}$.

Then $p_n(x) = \sum_{k=0}^{\infty} \beta_k \phi_k(x)$, and the normal equations become

$$\int_{a}^{b} w(x) \left(f(x) - \sum_{k=0}^{n} \beta_{k} \phi_{k}(x) \right) \phi_{i}(x) dx = 0 \text{ for } i = 0, 1, \dots, n,$$

or equivalently

$$\sum_{k=0}^{n} \left(\int_{a}^{b} w(x)\phi_{k}(x)\phi_{i}(x) dx \right) \beta_{k} = \int_{a}^{b} w(x)f(x)\phi_{i}(x) dx, \quad i = 0, \dots, n, \text{ i.e.,}$$

$$A\beta = \varphi, \tag{1}$$

where $\beta = (\beta_0, \beta_1, \dots, \beta_n)^T$, $\varphi = (f_1, f_2, \dots, f_n)^T$ and now

$$a_{i,k} = \int_a^b w(x)\phi_k(x)\phi_i(x) dx$$
 and $f_i = \int_a^b w(x)f(x)\phi_i(x) dx$.

So A is diagonal if

$$\langle \phi_i, \phi_k \rangle = \int_a^b w(x)\phi_i(x)\phi_k(x) dx \quad \begin{cases} = 0 & i \neq k \text{ and } \\ \neq 0 & i = k. \end{cases}$$

We can create such a set of **orthogonal polynomials**

$$\{\phi_0,\phi_1,\ldots,\phi_n,\ldots\},\$$

with $\phi_i \in \Pi_i$ for each i, by the Gram–Schmidt procedure, which is based on the following lemma.

Lemma. Suppose that ϕ_0, \ldots, ϕ_k , with $\phi_i \in \Pi_i$ for each i, are orthogonal with respect to the inner product $\langle f, g \rangle = \int_a^b w(x) f(x) g(x) dx$. Then,

$$\phi_{k+1}(x) = x^{k+1} - \sum_{i=0}^{k} \lambda_i \phi_i(x)$$

satisfies

$$\langle \phi_{k+1}, \phi_j \rangle = \int_a^b w(x)\phi_{k+1}(x)\phi_j(x) dx = 0, \quad j = 0, 1, \dots, k, \text{ with}$$

$$\lambda_j = \frac{\langle x^{k+1}, \phi_j \rangle}{\langle \phi_j, \phi_j \rangle}, \quad j = 0, 1, \dots, k.$$

Proof. For any j, $0 \le j \le k$,

$$\langle \phi_{k+1}, \phi_j \rangle = \langle x^{k+1}, \phi_j \rangle - \sum_{i=0}^k \lambda_i \langle \phi_i, \phi_j \rangle$$

$$= \langle x^{k+1}, \phi_j \rangle - \lambda_j \langle \phi_j, \phi_j \rangle$$
by the orthogonality of ϕ_i and ϕ_j , $i \neq j$,
$$= 0 \quad \text{by definition of } \lambda_j. \quad \Box$$

Notes: 1. The G–S procedure does this successively for k = 0, 1, ..., n.

- 2. ϕ_k is always of exact degree k, so $\{\phi_0, \ldots, \phi_\ell\}$ is a basis for $\Pi_\ell \ \forall \ell \geq 0$.
- 3. ϕ_k can be normalised to satisfy $\langle \phi_k, \phi_k \rangle = 1$ or to be monic, or ...

Examples: 1. The inner product $\langle f, g \rangle = \int_{-1}^{1} f(x)g(x) dx$

gives orthogonal polynomials called the Legendre polynomials,

$$\phi_0(x) \equiv 1$$
, $\phi_1(x) = x$, $\phi_2(x) = x^2 - \frac{1}{3}$, $\phi_3(x) = x^3 - \frac{3}{5}x$,...

2. The inner product $\langle f, g \rangle = \int_{-1}^{1} \frac{f(x)g(x)}{\sqrt{1-x^2}} dx$

gives orthogonal polynomials called the Chebyshev polynomials,

$$\phi_0(x) \equiv 1$$
, $\phi_1(x) = x$, $\phi_2(x) = 2x^2 - 1$, $\phi_3(x) = 4x^3 - 3x$,...

3. The inner product $\langle f, g \rangle = \int_0^\infty e^{-x} f(x) g(x) dx$

gives orthogonal polynomials called the Laguerre polynomials,

$$\phi_0(x) \equiv 1, \quad \phi_1(x) = 1 - x, \quad \phi_2(x) = 2 - 4x + x^2,$$

 $\phi_3(x) = 6 - 18x + 9x^2 - x^3, \dots$

Lemma. Suppose that $\{\phi_0, \phi_1, \dots, \phi_k, \dots\}$ are orthogonal polynomials for a given inner product $\langle \cdot, \cdot \rangle$. Then, $\langle \phi_k, q \rangle = 0$ whenever $q \in \Pi_{k-1}$.

Proof. This follows since if $q \in \Pi_{k-1}$, then $q(x) = \sum_{i=0}^{k-1} \sigma_i \phi_i(x)$ for some $\sigma_i \in \mathbb{R}$, $i = 0, 1, \ldots, k-1$, so

$$\langle \phi_k, q \rangle = \sum_{i=0}^{k-1} \sigma_i \langle \phi_k, \phi_i \rangle = 0.$$

Remark: note from the above argument that if $q(x) = \sum_{i=0}^{k} \sigma_i \phi_i(x)$ is of exact degree k (so $\sigma_k \neq 0$), then $\langle \phi_k, q \rangle = \sigma_k \langle \phi_k, \phi_k \rangle \neq 0$.

Theorem. Suppose that $\{\phi_0, \phi_1, \dots, \phi_n, \dots\}$ is a set of orthogonal polynomials. Then, there exist sequences of real numbers $(\alpha_k)_{k=1}^{\infty}$, $(\beta_k)_{k=1}^{\infty}$, $(\gamma_k)_{k=1}^{\infty}$ such that a three-term recurrence relation holds of the form

$$\phi_{k+1}(x) = \alpha_k(x - \beta_k)\phi_k(x) - \gamma_k\phi_{k-1}(x), \qquad k = 1, 2, \dots$$

Proof. The polynomial $x\phi_k \in \Pi_{k+1}$, so there exist real numbers

$$\sigma_{k,0}, \sigma_{k,1}, \ldots, \sigma_{k,k+1}$$

such that

$$x\phi_k(x) = \sum_{i=0}^{k+1} \sigma_{k,i}\phi_i(x)$$

as $\{\phi_0, \phi_1, \dots, \phi_{k+1}\}$ is a basis for Π_{k+1} . Now take the inner product on both sides with ϕ_j where $j \leq k-2$. On the left-hand side, note $x\phi_j \in \Pi_{k-1}$ and thus

$$\langle x\phi_k, \phi_j \rangle = \int_a^b w(x)x\phi_k(x)\phi_j(x) dx = \int_a^b w(x)\phi_k(x)x\phi_j(x) dx = \langle \phi_k, x\phi_j \rangle = 0,$$

by the above lemma for $j \leq k-2$. On the right-hand side

$$\left\langle \sum_{i=0}^{k+1} \sigma_{k,i} \phi_i, \phi_j \right\rangle = \sum_{i=0}^{k+1} \sigma_{k,i} \langle \phi_i, \phi_j \rangle = \sigma_{k,j} \langle \phi_j, \phi_j \rangle$$

by the linearity of $\langle \cdot, \cdot \rangle$ and orthogonality of ϕ_i and ϕ_j for $i \neq j$. Hence $\sigma_{k,j} = 0$ for $j \leq k-2$, and so

$$x\phi_k(x) = \sigma_{k,k+1}\phi_{k+1}(x) + \sigma_{k,k}\phi_k(x) + \sigma_{k,k-1}\phi_{k-1}(x).$$

Almost there: taking the inner product with ϕ_{k+1} reveals that

$$\langle x\phi_k, \phi_{k+1} \rangle = \sigma_{k,k+1} \langle \phi_{k+1}, \phi_{k+1} \rangle,$$

so $\sigma_{k,k+1} \neq 0$ by the above remark as $x\phi_k$ is of exact degree k+1 (e.g., from above Gram–Schmidt notes). Thus,

$$\phi_{k+1}(x) = \frac{1}{\sigma_{k,k+1}}(x - \sigma_{k,k})\phi_k(x) - \frac{\sigma_{k,k-1}}{\sigma_{k,k+1}}\phi_{k-1}(x),$$

which is of the given form, with

$$\alpha_k = \frac{1}{\sigma_{k,k+1}}, \qquad \beta_k = \sigma_{k,k}, \qquad \gamma_k = \frac{\sigma_{k,k-1}}{\sigma_{k,k+1}}, \qquad k = 1, 2, \dots$$

That completes the proof.

Example. The inner product $\langle f, g \rangle = \int_{-\infty}^{\infty} e^{-x^2} f(x) g(x) dx$

gives orthogonal polynomials called the Hermite polynomials,

$$\phi_0(x) \equiv 1$$
, $\phi_1(x) = 2x$, $\phi_{k+1}(x) = 2x\phi_k(x) - 2k\phi_{k-1}(x)$ for $k \ge 1$.

Listing 1: hermite_polys.m

```
1 %% Demonstrate Hermite Orthogonal Polynomials
  lw = 'linewidth';
x = linspace(-2.2, 2.2, 256);
  H_old = ones(size(x));
5 H = figure(1); clf;
6 plot(x, H_old, 'r-', lw,2)
  set(get(H,'children'), 'fontsize', 16);
8 hold on;
            pause
  H = 2*x;
  plot(x, H, lw,2, 'color',[0 0.75 0])
11
12
  for n = 1:4
14
    % use the three-term recurrence
    H_{new} = (2*x).*H - (2*n)*H_{old};
16
    plot(x, H_new, lw,2, 'color',rand(3,1))
17
    pause;
18
    H_old = H; H = H_new;
19
20
  legend('H_0(x)', 'H_1(x)', 'H_2(x)', 'H_3(x)', 'H_4(x)', 'H_5(x)')
21
  xlabel('x'); title('Hermite orthogonal polynomials')
```

