Numerical Analysis Hilary Term 2018
Lecture 12: 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 $\{1, x, x^2, \ldots, x^n\}$ as a basis for Π_n, suppose we have a basis $\{\phi_0, \phi_1, \ldots, \phi_n\}$. Then $p_n(x) = \sum_{k=0}^{n} \beta_k \phi_k(x)$, and the normal equations become

$$\int_a^b w(x) \left(f(x) - \sum_{k=0}^{n} \beta_k \phi_k(x) \right) \phi_i(x) \, \mathrm{d}x = 0 \quad \text{for} \quad i = 0, 1, \ldots, n,$$

or equivalently

$$\sum_{k=0}^{n} \left(\int_a^b w(x) \phi_k(x) \phi_i(x) \, \mathrm{d}x \right) \beta_k = \int_a^b w(x) f(x) \phi_i(x) \, \mathrm{d}x, \quad i = 0, \ldots, n, \quad \text{i.e.,}$$

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

where $\beta = (\beta_0, \beta_1, \ldots, \beta_n)^{\mathrm{T}}$, $\varphi = (f_1, f_2, \ldots, f_n)^{\mathrm{T}}$ and now

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

So A is diagonal if

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

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 $\phi_0, \ldots, \phi_k$, with $\phi_i \in \Pi_i$ for each i, are orthogonal with respect to the inner product $\langle f, g \rangle = \int_a^b w(x) f(x) g(x) \, \mathrm{d}x$. Then,

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

satisfies

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

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

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

$$\begin{aligned}\langle \phi_{k+1}, \phi_j \rangle = \;& \langle x^{k+1}, \phi_j \rangle - \sum_{i=0}^{k} \lambda_i \langle \phi_i, \phi_j \rangle \\ = \;& \langle x^{k+1}, \phi_j \rangle - \lambda_j \langle \phi_j, \phi_j \rangle \\ & \qquad \text{by the orthogonality of } \phi_i \text{ and } \phi_j,\ i \neq j, \\ = \;& 0 \qquad \text{by definition of } \lambda_j. \end{aligned}$$

□

Notes: 1. The G–S procedure does this successively for $k = 0, 1, \dots, n$.
2. ϕ_k is always of exact degree k, so $\{\phi_0, \dots, \phi_\ell\}$ is a basis for Π_ℓ $\forall \ell \ge 0$.
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 $\langle f, g \rangle = \displaystyle\int_{-1}^{1} f(x) g(x) \,\mathrm{d}x$

gives orthogonal polynomials called the **Legendre polynomials**,

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

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

gives orthogonal polynomials called the **Chebyshev polynomials**,

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

3. The inner product $\langle f, g \rangle = \displaystyle\int_{0}^{\infty} \mathrm{e}^{-x} f(x) g(x) \,\mathrm{d}x$

gives orthogonal polynomials called the **Laguerre polynomials**,

$$\phi_0(x) \equiv 1, \;\; \phi_1(x) = 1 - x, \;\; \phi_2(x) = 2 - 4x + x^2,$$
$$\phi_3(x) = 6 - 18x + 9x^2 - x^3, \dots$$

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 $q(x) = \displaystyle\sum_{i=0}^{k-1} \sigma_i \phi_i(x)$ for some $\sigma_i \in \mathbb{R}$, $i = 0, 1, \dots, k-1$, 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 $q(x) = \displaystyle\sum_{i=0}^{k} \sigma_i \phi_i(x)$ 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 $\{\phi_0, \phi_1, \ldots, \phi_{k+1}\}$ 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

$$\langle x\phi_k, \phi_j\rangle = \int_a^b w(x)x\phi_k(x)\phi_j(x)\,\mathrm{d}x = \int_a^b w(x)\phi_k(x)x\phi_j(x)\,\mathrm{d}x = \langle \phi_k, x\phi_j\rangle = 0,$$

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

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

That completes the proof. $\square$

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

gives orthogonal polynomials called the **Hermite polynomials**,

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

Listing 1: hermite_polys.m

```
%% Demonstrate Hermite Orthogonal Polynomials
lw = 'linewidth';
x = linspace(-2.2, 2.2, 256);
H_old = ones(size(x));
H = figure(1); clf;
plot(x, H_old, 'r-', lw,2)
set(get(H,'children'), 'fontsize', 16);
hold on;  pause

H = 2*x;
plot(x, H, lw,2, 'color',[0 0.75 0])
pause

for n = 1:4
  % use the three-term recurrence
  H_new = (2*x).*H - (2*n)*H_old;
  plot(x, H_new, lw,2, 'color',rand(3,1))
  pause;
  H_old = H;  H = H_new;
end
legend('H_0(x)', 'H_1(x)', 'H_2(x)', 'H_3(x)', 'H_4(x)', 'H_5(x)')
xlabel('x'); title('Hermite orthogonal polynomials')
```