Numerical Analysis Hilary Term 2025
Lecture 10: Orthogonal Polynomials

Recall from last lecture that, given an inner-product space V and a finite dimensional space W, we want to find the best approximation of $f \in V$ in W:

$$\|f - p\| \leq \|f - r\| \qquad \forall r \in W, \tag{1}$$

where $\|\cdot\|^2 := \langle \cdot, \cdot \rangle$ is the norm induced by the inner-product on V. The best approximation $p \in W$ satisfies the following orthogonality condition

$$\langle f - p, r \rangle = 0 \qquad \forall r \in W, \tag{2}$$

which can be expressed as a finite-dimensional linear system

$$A\alpha = \varphi, \tag{3}$$

where $\{\phi_k\}_{k=1}^{n=\dim W}$ is a basis for W, $p = \sum_{k=1}^{n} \alpha_k \phi_k$,

$$a_{i,k} = \langle \phi_k, \phi_i \rangle \quad \text{and} \quad \varphi_i = \langle f, \phi_i \rangle \, .$$

For the remainder of this lecture, we are most interested in the special case that $V = L^2_w(a,b)$ is the space of (weighted) square-integrable functions on (a,b) and $W = \Pi_m$ is the space of polynomials of degree $\leq m$.

Gram–Schmidt orthogonalization procedure

The solution of the normal equations $A\alpha = \varphi$ for best least-squares approximation would be easy if A were diagonal. Note that A is diagonal if

$$a_{i,k} = \langle \phi_k, \phi_i \rangle \begin{cases} = 0 & \text{if } i \neq k, \\ \neq 0 & \text{if } i = k. \end{cases}$$

We can create such an orthogonal basis by the Gram–Schmidt procedure:

Lemma. Let $\{\phi_k\}_{k=1}^{n}$ be a basis for W. Then, the set $\{\psi_k\}_{k=1}^{n} \subset W$ defined recursively by

$$\psi_1 := \phi_1 \quad \text{and} \quad \psi_{k+1} := \phi_{k+1} - \sum_{i=1}^{k} \frac{\langle \phi_{k+1}, \psi_i \rangle}{\langle \psi_i, \psi_i \rangle} \psi_i, \quad k = 1, 2, \ldots, n-1,$$

is orthogonal.

Proof. Let $k, j \in \{1, 2, \ldots, n\}$ with $j < k$. Then,

$$\begin{aligned} \langle \psi_k, \psi_j \rangle &= \langle \phi_k, \psi_j \rangle - \sum_{i=1}^{k-1} \frac{\langle \phi_k, \psi_i \rangle}{\langle \psi_i, \psi_i \rangle} \langle \psi_i, \psi_j \rangle \\ &= \langle \phi_k, \psi_j \rangle - \frac{\langle \phi_k, \psi_j \rangle}{\langle \psi_j, \psi_j \rangle} \langle \psi_j, \psi_j \rangle \qquad \text{[by orthogonality]} \\ &= 0. \end{aligned}$$

Thus, $\{\psi_k\}$ is orthogonal. □

So, we can solve the normal equations (3) we can

1. Perform Gram-Schmidt to transform our original basis $\{\phi_k\}$ for W to an orthogonal basis $\{\psi_k\}$.
2. Form the normal equations (3), which is diagonal.
3. Invert the diagonal system.

Lemma. Suppose that $\{\phi_1, \phi_2, \ldots, \phi_n\}$ is an orthogonal basis for W. Then, for any $w \in W$, there holds

$$w = \sum_{i=1}^{n} \frac{\langle w, \phi_i \rangle}{\langle \phi_i, \phi_i \rangle} \phi_i. \tag{4}$$

Proof. Since $\{\phi_1, \phi_2, \ldots, \phi_n\}$ is a basis for W, there exists $\sigma_1, \sigma_2, \ldots, \sigma_n$ such that $w = \sum_{i=1}^{n} \sigma_i \phi_i$. Taking the inner-product against ϕ_j and using linearity give

$$\langle w, \phi_j \rangle = \sum_{i=1}^{n} \sigma_i \langle \phi_i, \phi_j \rangle = \sigma_j \langle \phi_j, \phi_j \rangle .$$

Thus, $\sigma_j = \langle w, \phi_j \rangle / \langle \phi_j, \phi_j \rangle$, which completes the proof. $\square$

Lemma. Suppose that $\{\phi_1, \phi_2, \ldots, \phi_n\}$ is an orthogonal basis for W. Then, given $f \in V$, the element $p \in W$ defined by

$$p = \sum_{i=1}^{n} \frac{\langle f, \phi_i \rangle}{\langle \phi_i, \phi_i \rangle} \phi_i \tag{5}$$

satisfies (1).

Proof. This follows immediately from the previous lemma and (2). $\square$

Remark: The above result shows that if the basis $\{\phi_1, \phi_2, \ldots, \phi_n\}$ is orthogonal, then the system (3) can be inverted directly by computing $2n$ inner-products.

Orthogonal Polynomials

Applying Gram-Schmidt (and switching notation), we can create such a set of **orthogonal polynomials** with respect to the inner-product $\langle f, g \rangle = \int_a^b w(x) f(x) g(x) \, \mathrm{d}x$

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

with $\phi_i \in \Pi_i$ for each i, by applying Gram-Schmidt to monomials $\{1, x, \ldots, x^n, \ldots\}$:

$$\phi_0 := 1 \quad \text{and} \quad \phi_{k+1} := x^{k+1} - \sum_{i=0}^{k} \frac{\langle x^{k+1}, \phi_i \rangle}{\langle \phi_i, \phi_i \rangle} \phi_i, \quad k = 1, 2, \ldots . \tag{6}$$

Notes:

1. ϕ_k is always of exact degree k, so $\{\phi_0, \ldots, \phi_\ell\}$ is a basis for Π_ℓ $\forall \ell \geq 0$.
2. Here, we have normalized ϕ_k to be monic. Alternatively, we can normalize ϕ_k to be orthonormal $\langle \phi_k, \phi_k \rangle = 1$, to be 1 at $x = b$, or whatever normalization we want.

In general, we say that $\{\phi_0, \phi_1, \ldots, \phi_n, \ldots\}$ is a set of **orthogonal polynomials** with respect to an inner-product $\langle \cdot, \cdot \rangle$ if $\phi_i \in \Pi_i$ for all $i = 0, 1, \ldots$ and $\langle \phi_i, \phi_j \rangle = 0$ for all $i \neq j$.

Examples: (All normalized differently)

1. The inner product $\langle f, g \rangle = \int_{-1}^{1} f(x)g(x)\,\mathrm{d}x$ gives orthogonal polynomials called the **Legendre polynomials**:

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

2. The inner product $\langle f, g \rangle = \int_{-1}^{1} \frac{f(x)g(x)}{\sqrt{1-x^2}}\,\mathrm{d}x$ gives orthogonal polynomials called the **Chebyshev polynomials**:

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

3. The inner product $\langle f, g \rangle = \int_{0}^{\infty} e^{-x} f(x)g(x)\,\mathrm{d}x$ gives orthogonal polynomials called the **Laguerre polynomials**:

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

Lemma. Suppose that $\{\phi_0, \phi_1, \ldots, \phi_k, \ldots\}$ 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

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

which completes the proof. □

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

Lemma. Suppose that we apply Gram-Schmidt to a set $\{p_0, p_1, \ldots, p_n, \ldots\}$, where $p_i \in \Pi_i$ are monic:

$$\omega_0 := 1 \quad \text{and} \quad \omega_{k+1} := p_{k+1} - \sum_{i=0}^{k} \frac{\langle p_{k+1}, \omega_i \rangle}{\langle \omega_i, \omega_i \rangle} \omega_i, \quad k = 1, 2, \ldots. \tag{7}$$

Then, $\omega_k = \phi_k$ for all $k = 0, 1, \ldots,$ where $\{\phi_k\}$ are given by (6). That is, applying Gram-Schmidt to any set of monic polynomials results in the same set of orthogonal polynomials.

Proof. The case $i = 1$ is trivial, so suppose that $i \geq 2$. Since p_i is monic, ω_i is also monic, and so $e_i := \omega_i - \phi_i \in \Pi_{i-1}$. The above lemma shows that $\langle \omega_i, q \rangle = 0$ for all $q \in \Pi_{i-1}$, and so $\langle e_i, q \rangle = 0$ for all $q \in \Pi_{i-1}$. Thus, $e_i \equiv 0$. $\square$

Exercise: Prove the more general result: If $\{\phi_0, \phi_1, \ldots, \phi_n, \ldots\}$ and $\{\omega_0, \omega_1, \ldots, \omega_n, \ldots\}$ are two sets of orthogonal polynomials with respect to the same inner-product, then $\phi_i = c_i \omega_i$ with $c_i \neq 0$ for all i.

Note that computing the next orthogonal polynomial in (6) requires computing $2(k+1)$ inner-products (or $k+1$ if we store $\|\phi_i\|^2$ or $k+2$ if we normalize ϕ_i to have norm 1 at each step). For general inner-product spaces, the $\mathcal{O}(k)$ complexity cannot be improved. However, we will see how this complexity can be improved for L^2-orthogonal polynomials.

Recurrences for Orthogonal Polynomials

Suppose that instead of using x^{k+1} to compute ϕ_{k+1} in (6), we use the monic polynomials $p_{k+1} := x\phi_k \in \Pi_{k+1}$ in (7). By the previous lemma above, this produces the same orthogonal polynomials:

$$\phi_{k+1} = x\phi_k - \sum_{i=0}^{k} \frac{\langle x\phi_k, \phi_i \rangle}{\langle \phi_i, \phi_i \rangle} \phi_i.$$

Note that $x\phi_i \in \Pi_{i+1}$, and so the above lemma gives

$$\langle x\phi_k, \phi_i \rangle = \langle \phi_k, x\phi_i \rangle = 0 \quad \text{for } i = 0, 1, \ldots, k-2.$$

Consequently, we have

$$\phi_{k+1} = x\phi_k - \frac{\langle x\phi_k, \phi_k \rangle}{\langle \phi_k, \phi_k \rangle}\phi_k - \frac{\langle x\phi_k, \phi_{k-1} \rangle}{\langle \phi_{k-1}, \phi_{k-1} \rangle}\phi_{k-1} = \left(x - \frac{\langle x\phi_k, \phi_k \rangle}{\langle \phi_k, \phi_k \rangle} \right) \phi_k - \frac{\langle x\phi_k, \phi_{k-1} \rangle}{\langle \phi_{k-1}, \phi_{k-1} \rangle}\phi_{k-1}.$$

Conclusion: Using this particular set of monic polynomials, we only require $\mathcal{O}(1)$ inner-products to compute ϕ_{k+1} given $\phi_0, \phi_1, \ldots, \phi_k$. Overall, to solve the least squares problem (1) with $V = L^2_w(a, b)$ and $W = \Pi_n$, we first form an orthogonal basis $\{\phi_0, \phi_1, \ldots, \phi_n\}$ at a cost of $\mathcal{O}(n)$ inner-products and then construct p using (5) which takes an additional $\mathcal{O}(n)$ inner-products. While all seems good, we still need to compute the inner-products (integrals). The next lecture addresses how to do this accurately and efficiently.

The above recurrence relation is a particular case of the following more general result:

Theorem. Suppose that $\{\phi_0, \phi_1, \ldots, \phi_n, \ldots\}$ 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

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

Proof. Since the polynomial $x\phi_k \in \Pi_{k+1}$, so we can expand it in the orthogonal basis $\{\phi_0, \phi_1, \ldots, \phi_{k+1}\}$:

$$x\phi_k(x) = \sum_{i=0}^{k+1} \frac{\langle x\phi_k, \phi_i\rangle}{\|\phi_i\|^2}\phi_i(x)$$

Note that $x\phi_i \in \Pi_{i+1} \implies \sigma_{k,i} = 0$ for $i = 0, 1, \ldots, k-2$, and so

$$x\phi_k(x) = \frac{\langle x\phi_k, \phi_{k+1}\rangle}{\|\phi_{k+1}\|^2}\phi_{k+1}(x) + \frac{\langle x\phi_k, \phi_k\rangle}{\|\phi_k\|^2}\phi_k(x) + \frac{\langle x\phi_k, \phi_{k-1}\rangle}{\|\phi_{k-1}\|^2}\phi_{k-1}(x).$$

Now, $\langle x\phi_k, \phi_{k+1}\rangle \neq 0$ as $x\phi_k$ is of exact degree $k+1$ (e.g., from above notes). Thus,

$$\phi_{k+1}(x) = \frac{\|\phi_{k+1}\|^2}{\langle x\phi_k, \phi_{k+1}\rangle}\left(x - \frac{\langle x\phi_k, \phi_k\rangle}{\|\phi_k\|^2}\right)\phi_k(x) - \frac{\langle x\phi_k, \phi_{k-1}\rangle}{\langle x\phi_k, \phi_{k+1}\rangle}\frac{\|\phi_{k+1}\|^2}{\|\phi_{k-1}\|^2}\phi_{k-1}(x),$$

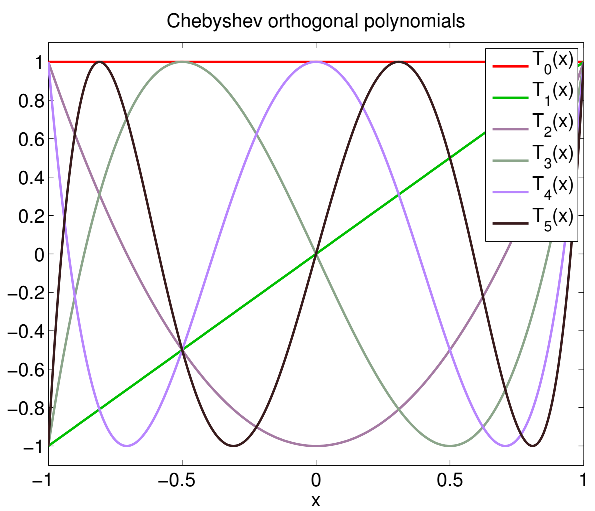
which is of the given form, with

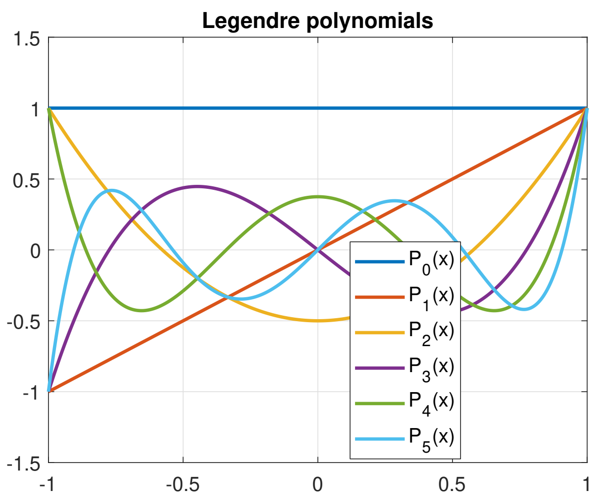
$$\alpha_k = \frac{\|\phi_{k+1}\|^2}{\langle x\phi_k, \phi_{k+1}\rangle}, \qquad \beta_k = \frac{\langle x\phi_k, \phi_k\rangle}{\|\phi_k\|^2}, \qquad \gamma_k = \frac{\langle x\phi_k, \phi_{k-1}\rangle}{\langle x\phi_k, \phi_{k+1}\rangle}\frac{\|\phi_{k+1}\|^2}{\|\phi_{k-1}\|^2}, \qquad k = 1, 2, \ldots,$$

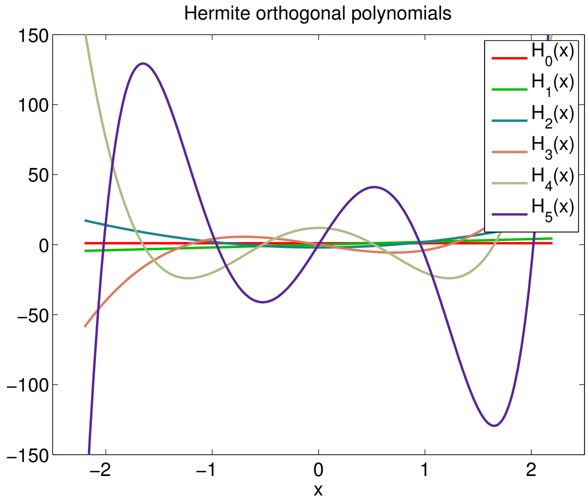
which completes the proof. $\square$

Example. The inner product $\langle f, g\rangle = \int_{-\infty}^{\infty} e^{-x^2} f(x)g(x)\,\mathrm{d}x$ gives orthogonal polynomials called the **Hermite polynomials**,

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






Hermite orthogonal polynomials
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x
$H_0(x)$
$H_1(x)$
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