Orthogonal Polynomials and the Gram–Schmidt Construction

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1. Functional Analytic Background

In quantum mechanics and mathematical physics, we often work within an inner product space of functions. A particularly important example is the weighted L^2 space:

$$L_w^2(a,b) = \left\{ f : (a,b) \to \mathbb{R} \;\middle|\; \int_a^b |f(x)|^2 w(x)\,dx < \infty \right\},$$

where $w(x) > 0$ is a given *weight function* on (a,b).

Inner Product and Orthogonality

The inner product between two functions f and g in $L_w^2(a,b)$ is defined by

$$\langle f, g \rangle = \int_a^b f(x)\,g(x)\,w(x)\,dx.$$

Two functions are said to be *orthogonal* if $\langle f, g \rangle = 0$. If, in addition, $\langle f, f \rangle = 1$, then f is said to be *normalized*. A collection of orthonormal functions $\{\phi_n(x)\}$ satisfies

$$\langle \phi_m, \phi_n \rangle = \delta_{mn}.$$

Such systems form the backbone of quantum mechanics: wavefunctions (or eigenfunctions) of Hermitian operators are orthogonal under an appropriate weight $w(x)$.

Motivation for Orthogonal Polynomials

The space of polynomials on (a,b) is infinite-dimensional and can be turned into a Hilbert space by introducing an inner product with a suitable weight function. An *orthogonal polynomial system* $\{p_n(x)\}$ is one that satisfies

$$\int_a^b p_n(x)\,p_m(x)\,w(x)\,dx = 0, \qquad n \neq m.$$

These families — such as Legendre, Hermite, and Laguerre polynomials — arise naturally as eigenfunctions of self-adjoint differential operators in Sturm–Liouville form, and therefore also form a complete basis for $L_w^2(a,b)$.

2. The Gram–Schmidt Orthogonalization Process

Idea of the Method

Suppose we start with the sequence of linearly independent monomials:

$$f_0(x) = 1, \quad f_1(x) = x, \quad f_2(x) = x^2, \quad \dots$$

and we wish to generate an orthogonal set $\{\phi_n(x)\}$ with respect to some weight $w(x)$ on (a, b).

The Gram–Schmidt process constructs each ϕ_n recursively as:

$$\phi_0 = f_0, \qquad \phi_k = f_k - \sum_{j=0}^{k-1} \frac{\langle f_k, \phi_j \rangle}{\langle \phi_j, \phi_j \rangle} \phi_j.$$

This guarantees orthogonality:

$$\langle \phi_i, \phi_j \rangle = 0 \quad \text{for all } i \neq j.$$

If we further normalize each ϕ_n by dividing by its norm, we obtain an orthonormal set.

Worked Example: Constructing Legendre Polynomials

Let us apply the Gram–Schmidt procedure to the monomials $1, x, x^2, \dots$ on the interval $[-1, 1]$ with the weight $w(x) = 1$. We define the inner product as

$$\langle f, g \rangle = \int_{-1}^{1} f(x) g(x)\, dx.$$

Step 1: Start with $f_0(x) = 1$.

$$\phi_0(x) = 1, \quad \langle \phi_0, \phi_0 \rangle = \int_{-1}^{1} 1\, dx = 2.$$

Normalized form:

$$P_0(x) = \frac{\phi_0}{\sqrt{2}} = \frac{1}{\sqrt{2}}.$$

Step 2: Next, $f_1(x) = x$. Subtract its projection on ϕ_0:

$$\langle f_1, \phi_0 \rangle = \int_{-1}^{1} x\, dx = 0.$$

So $\phi_1 = f_1 = x$. Then

$$\langle \phi_1, \phi_1 \rangle = \int_{-1}^{1} x^2\, dx = \frac{2}{3}.$$

Normalized:

$$P_1(x) = \sqrt{\frac{3}{2}}\, x.$$

Step 3: Now $f_2(x) = x^2$. Subtract projections on ϕ_0 and ϕ_1:

$$\phi_2 = f_2 - \frac{\langle f_2, \phi_0 \rangle}{\langle \phi_0, \phi_0 \rangle}\phi_0 - \frac{\langle f_2, \phi_1 \rangle}{\langle \phi_1, \phi_1 \rangle}\phi_1.$$

Compute:

$$\langle f_2, \phi_0 \rangle = \int_{-1}^{1} x^2\, dx = \frac{2}{3}, \quad \langle f_2, \phi_1 \rangle = \int_{-1}^{1} x^3\, dx = 0.$$

Thus

$$\phi_2 = x^2 - \frac{1}{3}.$$

Normalize:

$$\langle \phi_2, \phi_2 \rangle = \int_{-1}^{1} (x^2 - \tfrac{1}{3})^2 dx = \frac{8}{45}, \quad P_2(x) = \frac{3}{2\sqrt{2}}(x^2 - \tfrac{1}{3}) = \frac{1}{2}(3x^2 - 1).$$

Observation. The resulting P_0, P_1, and P_2 are the first three **Legendre polynomials**. Thus, Gram–Schmidt applied to $\{1, x, x^2, \dots\}$ with $w(x) = 1$ automatically generates the Legendre family.

Functional–Analytic Interpretation

This process is equivalent to constructing an orthogonal basis in $L^2[-1, 1]$. Each resulting polynomial $P_n(x)$ is an eigenfunction of a self-adjoint differential operator

$$\mathcal{L} = \frac{\mathrm{d}}{\mathrm{d}x}\left[(1 - x^2)\frac{\mathrm{d}}{\mathrm{d}x}\right].$$

That is,

$$\mathcal{L}P_n(x) + n(n+1)P_n(x) = 0.$$

Hence, Gram–Schmidt gives not only orthogonal functions but also the eigenbasis of $\mathcal{L}$, showing the deep connection between orthogonalization and operator theory.