Hermite, Legendre, and Laguerre: Orthogonal Polynomials

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Abstract

There are three types of special functions that we come across in elementary Quantum Mechanics during our search for a solution to the Schrodinger equation. They are all take the form of "orthogonal polynomials:" Hermite polynomials, Legendre polynomials (and associated Legendre functions), and Laguerre polynomials (and associated Laguerre polynomials). In this set of notes, I outline some of their properties (and how to construct them) and indicate how they are related to each other. Of course, all of this material can be found in textbooks and reference books on mathematical physics, some of which are listed at the end.

1 Common Properties

All of these polynomials, and also most special functions (like Bessel functions, which are not polynomials), satisfy and number of relations of the same general form. The polynomial in question is denoted $f_n(x)$, which means that it is an nth order polynomial of x. Derivatives with respect to x are denoted by a prime: $f'(x) = df/dx$.

1. They, of course, must satisfy an orthogonality condition. Orthogonality, unlike for vectors, means the following:

$$\int_a^b w(x) f_n(x) f_m(x) dx = \delta_{nm},$$

   where δ_{nm} is the Kronecker delta function, which is equal to 1 if $n = m$ and is 0 otherwise. The interval $[a, b]$ defines the domain of applicability for the polynomials. The factor $w(x)$ is the "weight function" for those particular polynomials.

2. They satisfy a second-order differential equation

$$g_2(x) f''_n(x) + g_1(x) f'_n(x) + a_n f_n(x) = 0,$$

   where $g_2(x)$ and $g_1(x)$ are independent of n and a_n is a constant depending only on n.

3. They satisfy a recurrence relation

$$f_{n+1}(x) = (a_n + xb_n)f_n(x) - c_n f_{n-1}(x)$$

4. They can be constructed from a Rodrigues formula

$$f_n(x) = \frac{1}{e_n w(x)} \left(\frac{d}{dx} \right)^n \{w(x)[g(x)]^n\},$$

where if the functions $w(x)$ and $g(x)$ are known, it is a simple matter (although perhaps painstaking) to differentiate n times to find the nth polynomial.

5. They can be defined throught a generating function

$$g(x, z) = \sum_{n=0}^{\infty} a_n f_n(x) z^n,$$

which means that they are the coefficients of a power series expansion of some function g. That function is called the "generating function."

2 Hermite Polynomials

Let us take Hermite polynomials first. We encounter these while solving the one-dimensional harmonic oscillator problem. You can rewrite the Schrodinger equation to find an equation that these functions satisfy

$$H_n''(x) + -2xH_n'(x) + 2nH_n(x) = 0.$$

The wave function is related to these polynomials

$$\psi_n(x) = A_n H_n(\xi) e^{-\xi^2/2}$$

where

$$\xi = \sqrt{\frac{m\omega}{\hbar}} x$$

And A_n is a normalization factor. The recurrence relation is

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$$

The Rodrigues formula is

$$H_n(x) = (-1)^n e^{x^2} \left(\frac{d}{dx} \right)^n e^{-x^2}.$$

Finally, the generating function is

$$e^{-z^2+2zx} = \sum_{n=0}^{\infty} \frac{z^n}{n!} H_n(x)$$

The orthogonality condition is

$$\int_{-\infty}^{\infty} \frac{e^{-x^2}}{\sqrt{\pi} 2^n n!} H_n(x) H_m(x) dx = \delta_{nm}$$

3 Laguerre Polynomials

Now we examine Laguerre polynomials. We encounter these while solving the radial part of the Schrodinger equation for the Coulomb potential energy. After factoring out certain asymptotic behaviors of the radial wave function, you can rewrite the Schrodinger equation to find an equation whose solutions are the associated Laguerre polynomials. The (regular) Laguerre polynomials satisfy

$$xL_n''(x) + (1-x)L_n'(x) + nL_n(x) = 0.$$

The wave function $R(r)$ is related to these polynomials. Because it is a radial wave function, the argument of the polynomials is restricted to be positive, $x \geq 0$. The recurrence relation is

$$(n+1)L_{n+1}(x) = (2n+1-x)L_n(x) - nL_{n-1}(x)$$

The Rodrigues formula is

$$L_n(x) = e^x \left(\frac{d}{dx}\right)^n e^{-x}x^n.$$

Finally, the generating function is

$$\frac{1}{1-z}e^{zx/(z-1)} = \sum_{n=0}^{\infty} z^n L_n(x)$$

The orthogonality condition is

$$\int_0^{\infty} e^{-x}L_n(x)L_m(x)dx = \delta_{nm}$$

4 Legendre Polynomials

Finally, we look at the Legendre polynomials. We encounter these while solving the angular part of the Schrodinger equation for any central potential. As before, we must factor out certain asymptotic behaviors of the wave function, and then we can rewrite the Schrodinger equation to find an equation whose solutions are the associated Legendre functions. The (regular) Legendre polynomials satisfy

$$(1-x^2)P_n''(x) + -2xP_n'(x) + n(n+1)P_n(x) = 0.$$

The wave function $\Theta(\theta)$ is related to these polynomials. Because the argument will be replaced by $\cos\theta$, the absolute value of the argument of these polynomials is restricted to be less than or equal to unity, $-1 \leq x \leq 1$. The recurrence relation is

$$(n+1)P_{n+1}(x) = 2(n+1)xP_n(x) - nP_{n-1}(x)$$

The Rodrigues formula is

$$P_n(x) = \frac{1}{2^n n!}\left(\frac{d}{dx}\right)^n (x^2-1)^n.$$

Finally, the generating function is

$$\left(1 - 2xz + z^2\right)^{-1/2} = \sum_{n=0}^{\infty} z^n P_n(x)$$

The orthogonality condition is

$$\int_{-1}^{1} \frac{2n+1}{2} P_n(x) P_m(x) dx = \delta_{nm}$$

5 Afterword

You can work with each of these sets of polynomials in the same way. If you know the two lowest, you can generate all of them with the recursion relations (You can, of course, obtain them all directly with the Rodrigues formulas). The orthogonality criteria are useful when making statements about certain physical properties. The generating function is useful in determining other properties of the polynomials, but this topic is more advanced.