Orthogonal Polynomials

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List of Orthogonal Polynomials

Legendre polynomials:

$$a = -1 \qquad b = 1 \qquad w(x) = 1 \qquad \mathcal{N}_m = \left(m + \tfrac{1}{2}\right)^{1/2}$$

$$P_0 = 1 \qquad P_1 = x \qquad P_2 = (3x^2 - 1)/2$$

$$P_3 = (5x^3 - 3x)/2 \qquad P_4 = (35x^4 - 30x^2 + 3)/8$$

E.g. Multipole expansions of charge density

Associated LP appear as solutions to QM rigid rotor

$$P_k^{(m)}(x) = (1 - x^2)^{m/2} \frac{d^m}{dx^m} P_k(x).$$

Laguerre polynomials:

$$a = 0 \qquad b = \infty \qquad w(x) = e^{-x} \qquad \mathcal{N}_m = 1$$

$$L_0 = 1 \qquad L_1 = -x + 1 \qquad L_2 = (x^2 - 4x + 2)/2$$

$$L_3 = (-x^3 + 9x^2 - 18x + 6)/6 \qquad L_4 = (x^4 - 16x^3 + 72x^2 - 96x + 24)/24$$

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Associated Laguerre polynomials:

$$a = 0 \qquad b = \infty \qquad w(x) = x^k e^{-x} \qquad \mathcal{N}_m^{(k)} = \sqrt{m!/(m+k)!}$$

$$L_0^{(k)} = 1 \quad L_1^{(k)} = -x + k + 1 \quad L_2^{(k)} = [x^2 - 2(k+2)x + (k+1)(k+2)]/2$$

$$L_3^{(k)} = [-x^3 + 3(k+3)x^2 - 3(k+2)(k+3)x + (k+1)(k+2)(k+3)]/6$$

$$L_4^{(k)} = [x^4 - 4(k+4)x^3 + 6(k+3)(k+4)x^2 - 4(k+2)(k+3)(k+4)x + (k+1)(k+2)(k+3)(k+4)]/24$$

E.g. Solutions to radial Schrodinger equation of H atom

Hermite polynomials:

$$a = -\infty \qquad b = \infty \qquad w(x) = e^{-x^2} \qquad \mathcal{N}_m = (-1)^m 2^{-m/2} \pi^{-1/4} (m!)^{-1/2}$$

$$H_0 = 1 \qquad H_1 = 2x \qquad H_2 = 4x^2 - 2$$

$$H_3 = 8x^3 - 12x \qquad H_4 = 16x^4 - 48x^2 + 12$$

E.g. Solutions to Quantum Simple harmonic Oscillator

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Chebyschev polynomials of the first kind:

$a = -1 \quad b = 1 \quad w(x) = (1 - x^2)^{-1/2} \quad \mathcal{N}_0 = \sqrt{1/\pi} \quad \mathcal{N}_{m>0} = \sqrt{2/\pi}$

$T_0 = 1 \quad T_1 = x \quad T_2 = 2x^2 - 1 \quad T_3 = 4x^3 - 3x \quad T_4 = 8x^4 - 8x^2 + 1$

Chebyschev polynomials of the second kind:

$a = -1 \quad b = 1 \quad w(x) = (1 - x^2)^{1/2} \quad \mathcal{N}_m = \sqrt{2/\pi}$

$U_0 = 1 \quad U_1 = 2x \quad U_2 = 4x^2 - 1 \quad U_3 = 8x^3 - 4x \quad U_4 = 16x^4 - 12x^2 + 1$

Explicit expressions

$$L_m^{(k)}(x) = \sum_{j=0}^{m} (-1)^j \binom{m+k}{m-j} \frac{1}{j!} x^j , \quad \mathcal{L}_m^{(k)} = \sqrt{m!/(m+k)!}\, L_m^{(k)} , \tag{17.23}$$

$$H_m(x) = \sum_{j=0}^{[m/2]} \frac{(-1)^j m!}{j!(m-2j)!} (2x)^{m-2j} , \quad \mathcal{H}_m = (-1)^m 2^{-m/2} (m!)^{-1/2} \pi^{-1/4} H_m , \tag{17.24}$$

$$T_m(x) = \frac{m}{2} \sum_{j=0}^{[m/2]} (-1)^j \frac{(m-j-1)!}{j!(m-2j)!)} (2x)^{m-2j} ,$$

$$\mathcal{T}_0 = \sqrt{1/\pi} , \quad \mathcal{T}_{m>0} = \sqrt{2/\pi}\, T_m , \tag{17.25}$$

$$U_m(x) = \sum_{j=0}^{[m/2]} (-1)^j \frac{(m-j)!}{j!(m-2j)!} (2x)^{m-2j} , \quad \mathcal{U}_m = \sqrt{2/\pi}\, U_m . \tag{17.26}$$

Explicit expressions

Table 17.2: Recursion relations for orthogonal polynomials.

$$(m+1)P_{m+1}(x) = (2m+1)xP_m(x) - mP_{m-1}(x)$$

$$(m+1)L_{m+1}^{(k)}(x) = (1+2m+k-x)L_m^{(k)} - (m+k)L_{m-1}^{(k)}$$

$$L_m^{(k+1)} = L_m^{(k)} + L_{m-1}^{(k-1)}$$

$$H_{m+1}(x) = 2xH_m(x) - 2mH_{m-1}(x)$$

$$T_{m+1}(x) = 2xT_m(x) - T_{m-1}(x)$$

$$U_{m+1}(x) = 2xU_m(x) - U_{m-1}(x)$$

Explicit expressions

Table 17.3: Differential equations satisfied by orthogonal polynomials.

P_m:	$(1-x^2)y'' - 2xy' + m(m+1)y = 0$
$L_m^{(k)}$:	$xy'' + (k+1-x)y' + my = 0$
H_m:	$y'' - 2xy' + 2my = 0$
T_m:	$(1-x^2)y'' - xy' + m^2y = 0$
U_m:	$(1-x^2)y'' - 3xy' + m(m+2)y = 0$

Function Resolution in O.P.

Definition. $C[a,b]$ is the Hilbert space that contains all functions that are continuous for all x in a finite interval $a \leq x \leq b$, over the field $\mathbb{C}$ and with inner product $\langle f, g\rangle = \int_a^b f^* g \, dx$.

Theorem 17.2.1. *(Weierstrass[7] approximation theorem) Any function in $C[a,b]$ can be approximated to arbitrarily high accuracy by a polynomial.*

It follows that $\{1, x, x^2, x^3, \ldots\}$ is a basis for $C[a,b]$. Any $f \in C[a,b]$ can be expressed as

$$f(x) \approx \sum_{k=0}^{N} a_k x^k \qquad (17.27)$$

Function Resolution in O.P.

Definition. L^2 is the Hilbert space that contains all piecewise-continuous[8] functions f such that $\langle f, f\rangle$ is finite, with inner product $\langle f, g\rangle = \int_{-\infty}^{\infty} f^* g\, dx$ and field $\mathbb{C}$. The functions in L^2 are said to be ***square integrable***. If the inner product contains a weight function, the space is called a *weighted* L^2 space, indicated with the notation $L^2[w(x)]$. If the range of integration in the inner product is $a \leq x \leq b$, then the space is designated $L^2[a, b; w(x)]$.

Turns out Weierstrass Approximation Theorem can be extended to L^2 functions as well.

References

Mathematical Methods for Physical and Analytical Chemistry

- David Z. Goodson