Series Solutions and Special Functions

Legendre Polynomials

A differential equation which is frequently encountered in physical problems with spherical geometry, with an angular dependence on the polar angle θ, is the Legendre equation

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + k\Theta = 0 \qquad \textbf{(1)}$$

in which k is a constant. Commonly this equation arises from a partial differential equation involving the Laplacian in spherical coordinates, in which case k comes from the process of separating the partial differential equation into ordinary differential equations.

It is convenient to make a substitution x = cosθ before solving Legendre's equation, in which case the differential equation takes on the form

$$(1 - x^2)\frac{d^2\Theta}{dx^2} - 2x\frac{d\Theta}{dx} + k\Theta = 0 \qquad \textbf{(2)}$$

This equation can be solved by finding the series solution of the form $\Theta = x^c (a_0 + a_1x + a_2x^2 + ...) = \Sigma\, a_n x^{c+n}$. Using standard techniques for finding series solution we get the indicial equation c(c-1)=0 and the recurrence relationship

$$(c+n+1)(c+n+2)\, a_{n+2} = \{(c+n)(c+n+1)-k\}\, a_n$$

The series solution therefore consists of an infinite number of terms which are all even (c=0) or all odd (c=1).

The infinite series solution is divergent when θ=0 or π (x=±1). To avoid this divergence we impose the condition that the series must terminate after a finite number of terms, which in turn requires that k must have the value $\ell(\ell+1)$ where ℓ (equal to c+n) is any positive integer, including zero. For each value of ℓ it is a simple task to use the recurrence relationship above to generate the appropriate series in x=cosθ. The first six Legendre polynomials $P_\ell(x)$ are given in the table to the right.

Legendre polynomials

$P_0(x) = 1$
$P_1(x) = x$
$P_2(x) = ½(3x^2 - 1)$
$P_3(x) = ½(5x^3 - 3x)$
$P_4(x) = ⅛(35x^4 - 30x^2 +3)$
$P_5(x) = ⅛(63x^5 - 70x^3 +15x)$

Orthonormality Property of Legendre Polynomials

There are a number of important properties of Legendre polynomials, especially the orthogonality condition

$$\int_0^{\pi} P_l(\theta)\, P_m(\theta) \sin\theta \, d\theta \;=\; \int_{-1}^{+1} P_l(x)\, P_m(x)\, dx \;=\; 0 \qquad \textbf{(3)}$$

if $\ell \neq m$. This condition allows the use of the Legendre polynomials as the basis set for solving problems with spherical symmetry using Fourier series. If $\ell = m$ then the normalization condition is

$$\int_0^{\pi} P_l^2(\theta) \sin\theta \, d\theta \;=\; \int_{-1}^{+1} P_l^2(x)\, dx \;=\; \frac{2}{2l+1} \qquad \textbf{(4)}$$

Recurrence relationship between Legendre Polynomials of different order

A useful recurrence relationship relates Legendre Polynomials of different order

$$P_{\ell+1}(x) \;=\; \frac{(2\ell+1)\, x\, P_\ell(x) \;-\; \ell\, P_{\ell-1}(x)}{\ell + 1} \qquad \textbf{(5)}$$

With the definition of the first two Legendre polynomials, $P_0(x)=1$ and $P_1(x)=x$, by successive application of this recurrence relationship an explicit polynomial representation of any higher order Legendre polynomial can be found. The Maple script to the right calculates and displays the Legendre polynomials up to $P_6(x)$.

Recurrence relationship

The first line defines an array for the Legendre polynomials up to P_6, and defines P_0 and P_1. The next line calculates P_2 through P_6. Change the value of N in the first line to calculate more (or fewer) polynomials.

```
> N:=6: P:=array[0..N]: P[0]:=1: P[1]:=x:
> for i from 1 to N-1 do
> P[i+1]:=((2*i+1)*x*P[i]-(i)*P[i-1])/(i+1)
> od:
```

The next line will print out P_i, for any defined value of i

```
> collect(P[i],x);
```

Note the use of the collect(f,x) function to collect terms in powers of x. Alternatively, you can print out all the polynomials up to P_N

```
> for i from 0 to N do collect(P[i],x) od;
```

Associated Legendre Polynomials and Spherical Harmonics

If a problem with spherical geometry has a solution which depends on both the polar angle θ and the azimuthal angle φ, then the differential equation has the form

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial Y}{\partial\theta} \right) \;+\; \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial^2\varphi} \;+\; k\,Y \;=\; 0 \qquad \textbf{(6)}$$

The first step in this solution of this equation is the separation of variables, that is to write $Y(\theta,\varphi) = \Theta(\theta)\Phi(\varphi)$ and split the above partial differential equations into two ordinary differential equations

$$\sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta} \right) \;+\; k \sin^2\theta\, \Theta \;-\; m^2\, \Theta \;=\; 0 \qquad \textbf{(7)}$$

and

$$\frac{d^2\Phi}{d\varphi^2} = -m^2\,\Phi \tag{8}$$

Equation (8) has the straightforward solution $\Phi = e^{im\varphi}$. Since this function should remain unchanged following one full circle around the z axis ($\varphi \rightarrow \varphi+2\pi$) the arbitrary constant (m) must be an integer.

Equation (6) is the defining equation for the associated Legendre polynomial. If m=0 this reduces to the same as equation (2), and has the same solution. For $m\neq 0$ the series solution produced from equation (6) has a different form. On physical grounds we shall again impose the condition that the series should be finite for $\theta=0$ or π, which as before requires that the series terminate with a finite number of terms. This requires two separate conditions, that $k=\ell(\ell+1)$ where $\ell\geq 0$ is an integer, and that $|m|\leq\ell$. A few associated Legendre polynomials are given in the table below.

Associated Legendre Polynomials $P_\ell^{|m|}$			
	m = 0	m = ±1	m = ±2
$\ell = 0$	$(1/4\pi)^{1/2}$	-	-
$\ell = 1$	$(3/4\pi)^{1/2}\cos\theta$	$(3/8\pi)^{1/2}\sin\theta$	-
$\ell = 2$	$(5/16\pi)^{1/2}(3\cos^2\theta - 1)$	$(15/8\pi)^{1/2}\sin\theta\cos\theta$	$(15/32\pi)^{1/2}\sin^2\theta$

With these associated Legendre polynomials from the table above the solution to equation (5) can be written as

$$Y_{\ell,|m|}(\theta,\varphi) = P_\ell^{|m|}(\theta)\, e^{im\varphi}$$

which are known as spherical harmonics. (The numerical factors in the associated Legendre polynomials are derived from the normalization condition $\int Y^*_{\ell,|m|} Y_{\ell,|m|} \sin\theta\, d\theta\, d\varphi = 1$ when the limits of integration are $\theta=0$ to π and $\varphi=0$ to 2π.)

Bessel Functions

Bessel functions are frequently encountered in problems which involve cylindrical geometry, arising from a partial differential equation involving the Laplacian in cylindrical coordinates. After separation the radial equation becomes

$$x^2\frac{d^2P}{dr^2} + r\frac{dP}{dr} + (r^2 - n^2)\,P = 0 \tag{9}$$

where n is a constant, usually with the condition that it be an integer because of boundary conditions found in the angular (φ) portion of the original partial differential equation.

The solution of equation (9) is an infinite polynomial in r, with the first term of order r^n

$$P = r^n (a_0 + a_1 r + a_2 r^2 + ...) = \Sigma\, a_i\, r^{n+i}$$

Using standard techniques for finding series solution we get the recurrence equation

$$a_i = \frac{a_{i-2}}{n^2 - (n+i)^2} = -\frac{a_{i-2}}{i(2n+i)}$$

For any given integer n, the infinite series which is produced by this recurrence relationship is known as the Bessel function $J_n(r)$. It is defined for both positive and negative values of n, with the relationship

$$J_{-n}(r) = (-1)^n J_n(r)$$

Since the Bessel equation (9) is a second order differential equation there must be two independent solutions. The second is the Neumann function, also known as the Bessel function of the second kind
$Y_n(r)$. However, this function diverges as $r \rightarrow 0$, and so it readily eliminated from most problems on physical grounds.

Zeroes of the Bessel function

The Bessel function is oscillatory, with a period that is roughly constant. The first five values of r for which $J_n(r)=0$ are given in the table below.

n=0	2.405	5.520	8.654	11.79	14.93
n=1	3.832	7.016	10.17	13.32	16.47
n=2	5.136	8.417	11.62	14.80	17.96
n=3	6.380	9.761	13.02	16.22	19.41
n=4	7.588	11.06	14.37	17.62	20.83
n=5	8.771	12.34	15.70	18.98	22.22

Hermite Polynomials

Hermite polynomials are usually first encountered in quantum mechanics when solving the differential equation (Schrodinger equation) for the simple harmonic oscillator with a potential $V=\frac{1}{2}m\omega_o^2x^2$. After redefining the variables Schrodinger's equation becomes

$$-\frac{d^2\psi}{dx^2} + x^2\psi = 2\varepsilon\psi \tag{11}$$

where $\varepsilon = E/\hbar\omega_o$ with E the energy of the oscillator. (This equation is commonly referred to as Weber's equation.) It has the solution $\psi = AH_n(x)\, e^{-\frac{1}{2}x^2}$, where the functions $H_n(x)$ are known as Hermite Polynomials and A is a normalizing constant (see below). By directly substituting in equation (11) it is found that the Hermite polynomials must satisfy the differential equation

$$\frac{d^2H_n}{dx^2} - 2x\frac{dH_n}{dx} + (2\varepsilon - 1)H_n = 0 \tag{12}$$

As before we will try to solve this equation to find H_n as a polynomial in x

$$H_n = x^n (a_0 + a_1 x + a_2 x^2 + ...) = \Sigma\, a_i\, x^{n+i}$$

Using standard techniques for finding series solution we get the recurrence equation

$$a_{n+2} = \frac{2n + 1 - 2\varepsilon}{(n+1)(n+2)}\, a_n$$

The infinite series diverges as $x\to\pm\infty$, forcing us to make sure that the series terminates after a finite number of terms ($a_{n+2}=0$). This requires that $\varepsilon=n+\frac{1}{2}$ for some value of n. The finite series that is produced is the Hermite polynomial. The first six Hermite polynomials are given in the table to the right.

The coefficients of the different terms in x have been chosen so that the wavefunction $\psi_n=AH_n(x)e^{-\frac{1}{2}x^2}$ with the constant A set equal to $(1/2^n n!\sqrt{\pi})^{\frac{1}{2}}$ is normalized, that is so that

$$\int_{-\infty}^{\infty} \psi_n^* \psi_n\, dx = \frac{1}{2^n n! \sqrt{\pi}} \int_{-\infty}^{\infty} H_n^2 e^{-x^2} dx = 1$$

Hermite Polynomials

$H_0(x) = 1$
$H_1(x) = 2x$
$H_2(x) = 4x^2 - 2$
$H_3(x) = 8x^3 - 12x$
$H_4(x) = 16x^4 - 48x^2 + 12$
$H_5(x) = 32x^5 - 160x^3 + 120x$

Hermite Polynomials and Maple

Hermite polynomials in Maple are contained in the library 'orthopoly', which should be loaded first. After that H(n,x) gives the Hermite polynomial $H_n(x)$

```
> with(orthopoly):
> H(5,x);
        32x^5 - 160x^3 + 120x
```

There is a recurrence relationship for the Hermite polynomials. With $H_0= 1$ and $H_1 = 2x$, for $n\geq 2$

$$H_n(x) = 2xH_{n-1}(x) - 2(n-1)H_{n-2}(x)$$

Laguerre Polynomials

The solution of the radial part of the wavefunction for the Hydrogen atom is the Laguerre Polynomial.

Starting with the Schrodinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi - \frac{e^2}{4\pi\varepsilon_o r}\psi = E\psi$$

in spherical polar coordinates; separating the equation in radial, polar, and azimuthal portions; and substituting a change of variable, we get the radial equation

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{dR}{d\rho}\right) + \left[\frac{n}{\rho} - \frac{l(l+1)}{\rho^2} - \frac{1}{4}\right]R = 0$$

where $\rho = \alpha r$, $\alpha^2 = -8mE/\hbar^2$, and $n = 2me^2/\alpha^2$. (I'll leave the details for Phys 4510, QMI!)

The solution of the radial equation is written in the form

$$R = e^{-\rho/2}\rho^l \Sigma a_i \rho^i$$

The summation part of this expression is known as a Laguerre polynomial, with the recursion relationship

$$a_{i+2} = \frac{n - (l+i+1)}{2(i+1)(l+1) + i(i+1)} a_i$$

The first few polynomials are given in the box to the right.

Laguerre Polynomials

$L_0(x) = 1$
$L_1(x) = 1-x$
$L_2(x) = 1 - 2x + x^2/2$
$L_3(x) = 1 - 3x + 3x^2/2 - x^3/6$
$L_4(x) = 1 - 4x + 3x^2 - 2x^3/3 + x^4/24$

Laguerre Polynomials and Maple

Laguerre polynomials in Maple are contained in the library 'orthopoly', which should be loaded first. After that L(n,x) gives the Laguerre polynomial $L_n(x)$

```
> with(orthopoly):
> L(3,x);
          1- 3x + 3x^2/2 - x^3/6
```