Chapter 5

Special Functions and Gaussian Quadrature

5.1 Special Functions and Recurrence Relations

Variables of Laplace equation $\nabla^2\Psi(\vec{r}) = 0$ in 3-dimension are separable, i.e.,

$$\begin{aligned}
\nabla^2\Psi(\vec{r}) &= \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right] X(x)Y(y)Z(z) \\
&= \left[\frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)\right]\frac{U(r)}{r}P(\theta)\Phi(\varphi) \\
&= \left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2}\right] R(\rho)\Phi(\varphi)Z(z) = 0. \qquad (5.1)
\end{aligned}$$

The differential equation of each component in a rectangular coordinate system becomes either $\left[\frac{d^2}{dx^2} + k^2\right] X(x) = 0$ with a real k,

$$\begin{aligned}
X(x) &= A\cos(kx+\alpha) = A\sin(kx+\beta) = A'\cos(kx) + B'\sin(kx) \\
&= Ce^{ikx} + C^* e^{-ikx}, \qquad (5.2)
\end{aligned}$$

or $\left[\frac{d^2}{dz^2} - \kappa^2\right] Z(z) = 0$ with a real κ,

$$Z(z) = Ae^{\kappa z} + Be^{-\kappa z}. \qquad (5.3)$$

For azimuthal angle φ dependent part, $\left[\frac{d^2}{d\varphi^2}+m^2\right]\Phi(\varphi)=0$ with a real m,

$$\Phi(\varphi) = Ae^{im\varphi}+Be^{-im\varphi}. \tag{5.4}$$

If $0\leq\varphi\leq 2\pi$, m should be an integer for $\Phi(\varphi)$ to be a single valued function. For radial part in a spherical polar coordinate system, $\left[\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}\right]U(r)=0$,

$$U(r) = Ar^{l+1}+Br^{-l}. \tag{5.5}$$

For polar angle θ dependent part,

$$\left[\frac{1}{\sin\theta}\frac{d}{d\theta}\sin\theta\frac{d}{d\theta}+\left(l(l+1)-\frac{m^2}{\sin^2\theta}\right)\right]P(\theta) = 0, \tag{5.6}$$

which becomes a generalized Legendre equation with $x=\cos\theta$. For radial part in a cylindrical polar coordinate system,

$$\left[\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}+\left(\kappa^2-\frac{\nu^2}{\rho^2}\right)\right]R(\rho) = 0, \tag{5.7}$$

which becomes a Bessel equation with $x=\kappa\rho$. The solutions form a complete set of orthogonal functions for the corresponding variables and has some recursion relations.

For a system with azimuthal symmetry, the differential equation for the polar angle θ becomes Legendre equation with $m=0$;

$$\frac{d}{dx}\left[(1-x^2)\frac{dP_l(x)}{dx}\right]+l(l+1)P_l(x) = 0 \tag{5.8}$$

with $-1\leq x=\cos\theta\leq 1$. The solution $P_l(x)$ is a Legendre polynomial of order l:

$$\begin{aligned}
P_0(x) &= 1,\\
P_1(x) &= x,\\
P_2(x) &= \frac{1}{2}(3x^2-1),\\
P_3(x) &= \frac{1}{2}(5x^3-3x),\\
P_4(x) &= \frac{1}{8}(35x^4-30x^2+3),\\
&\vdots
\end{aligned} \tag{5.9}$$

with the orthogonality condition of

$$\int_{-1}^{1} P_{l'}(x)P_l(x)dx = \frac{2}{2l+1}\delta_{l'l}. \tag{5.10}$$

Some recurrence relations of the Legendre polynomial are

$$(l+1)P_{l+1} - (2l+1)xP_l + lP_{l-1} = 0, \tag{5.11}$$

$$\frac{dP_{l+1}}{dx} - \frac{dP_{l-1}}{dx} - (2l+1)P_l = 0, \tag{5.12}$$

$$\frac{dP_{l+1}}{dx} - x\frac{dP_l}{dx} - (l+1)P_l = 0, \tag{5.13}$$

$$(x^2-1)\frac{dP_l}{dx} - lxP_l + lP_{l-1} = 0. \tag{5.14}$$

The solution of the generalized Legendre equation with $m \neq 0$ $(-1 \leq x \leq 1)$,

$$\frac{d}{dx}\left[(1-x^2)\frac{dP_l^m(x)}{dx}\right] + \left[l(l+1) - \frac{m^2}{1-x^2}\right]P_l^m(x) = 0, \tag{5.15}$$

is called an associated Legendre function $P_l^m(x)$:

$$P_l^m(x) = (-1)^m(1-x^2)^{m/2}\frac{d^m}{dx^m}P_l(x). \tag{5.16}$$

Spherical harmonics is defined by

$$Y_{lm}(\theta,\varphi) = \sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)e^{im\varphi}. \tag{5.17}$$

The orthonormality condition is

$$\int_0^{\pi}\sin\theta d\theta\int_0^{2\pi}d\varphi Y^*_{l'm'}(\theta,\varphi)Y_{lm}(\theta,\varphi) = \delta_{l'l}\delta_{m'm}. \tag{5.18}$$

The completeness relation is

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y^*_{lm}(\theta',\varphi')Y_{lm}(\theta,\varphi) = \delta(\cos\theta-\cos\theta')\delta(\varphi-\varphi'). \tag{5.19}$$

The differential equation for the cylindrical radius ρ with $0 \leq x = \kappa\rho$ is the Bessel differential equation;

$$\frac{d^2R_\nu(x)}{dx^2} + \frac{1}{x}\frac{dR_\nu(x)}{dx} + \left(1-\frac{\nu^2}{x^2}\right)R_\nu(x) = 0. \tag{5.20}$$

The solutions of this equation are the Bessel function $J_\nu(x)$ and Neumann function (Bessel function of the second kind) $N_\nu(x)$;

$$J_\nu(x) = \left(\frac{x}{2}\right)^\nu \sum_{j=0}^{\infty} \frac{(-1)^j}{j!\Gamma(j+\nu+1)} \left(\frac{x}{2}\right)^{2j}, \tag{5.21}$$

$$N_\nu(x) = \frac{J_\nu(x)\cos\nu\pi - J_{-\nu}(x)}{\sin\nu\pi}. \tag{5.22}$$

Hankel functions, Bessel function of the third kind, are defined as

$$\begin{aligned} H_\nu^{(1)}(x) &= J_\nu(x) + iN_\nu(x), \\ H_\nu^{(2)}(x) &= J_\nu(x) - iN_\nu(x). \end{aligned} \tag{5.23}$$

These Bessel functions all satisfy the recursion formulae

$$R_{\nu-1}(x) + R_{\nu+1}(x) = \frac{2\nu}{x} R_\nu(x), \tag{5.24}$$

$$R_{\nu-1}(x) - R_{\nu+1}(x) = 2\frac{dR_\nu(x)}{dx}. \tag{5.25}$$

If $\kappa^2 = -k^2 < 0$ in Eq.(5.7), then the differential equation becomes

$$\frac{d^2R_\nu(x)}{dx^2} + \frac{1}{x}\frac{dR_\nu(x)}{dx} - \left(1 + \frac{\nu^2}{x^2}\right) R_\nu(x) = 0 \tag{5.26}$$

with $x = k\rho$. The solutions of this equation are modified Bessel functions;

$$\begin{aligned} I_\nu(x) &= i^{-\nu} J_\nu(ix), \\ K_\nu(x) &= \frac{\pi}{2} i^{\nu+1} H_\nu^{(1)}(ix). \end{aligned} \tag{5.27}$$

For Poisson equation $\nabla^2\Psi(\vec{r}) = -k^2\Psi(\vec{r})$ or for time independent Schrödinger equation, the radial part of differential equation in a spherical coordinate system becomes

$$\frac{d^2R(r)}{dr^2} + \frac{2}{r}\frac{dR(r)}{dr} + \left[k^2 - \frac{l(l+1)}{r^2}\right] R(r) = 0, \tag{5.28}$$

compared to Eq.(5.7) of a Laplace equation in a cylindrical coordinate system. With $x = kr$, this becomes

$$\frac{d^2R_\nu(x)}{dx^2} + \frac{2}{x}\frac{dR_\nu(x)}{dx} + \left[1 - \frac{l(l+1)}{x^2}\right] R_\nu(x) = 0 \tag{5.29}$$

and the solutions are the spherical Bessel functions;

$$j_l(x) = \sqrt{\frac{\pi}{2x}} J_{l+1/2}(x), \tag{5.30}$$

$$n_l(x) = \sqrt{\frac{\pi}{2x}} N_{l+1/2}(x). \tag{5.31}$$

To evaluate the value of special function, we may use the corresponding recursion relation starting from the values of the lowest order. Using the recurrence formula of Eq.(5.11), we may evaluate the value of $P_l(x)$ of order l starting from the value of $P_0(x)$ and $P_1(x)$ for a given value of x. Similarly the value of Bessel function of order ν can be found using the recurrence relation Eq.(5.24) starting from $R_0(x)$ and $R_1(x)$. The recursion relation can also be used to evaluate the differential of the special function.

5.2 Gaussian Quadrature; Integral using Special Function

The form of N point numerical integrals in Sect.2.4 are

$$\int_{-1}^{1} f(x)dx \approx \sum_{n=1}^{N} w_n f(x_n). \tag{5.32}$$

As an example, for Simpson's rule of Eq.(2.20),

$$\begin{array}{lll} x_1 = -1, & x_2 = 0, & x_3 = 1; \\ w_1 = 1/3, & w_2 = 4/3, & w_3 = 1/3 \end{array} \tag{5.33}$$

with $N = 3$. For N point integral with equally spaced points, Eq.(5.32) is exact for a polynomial $f(x)$ of order $(N-1)$. Thus the weighting factor w_n can be found from the conditions of

$$\int_a^b x^p dx = \left.\frac{x^{p+1}}{p+1}\right|_a^b = \sum_{n=1}^{N} w_n x_n^p \; ; \quad p = 0, 1, \cdots, (N-1). \tag{5.34}$$

Notice here that x_n does not need to be equally spaced in general.

If we determine x_n together with w_n for N points by condition of Eq.(5.34) with $p = 0, 1, \cdots, (2N-1)$, then Eq.(5.32) is exact for $(2N-1)$-th order polynomial $f(x)$. The x_n can also be determined by using special function.

As an example for integral range of $[a, b] = [-1, 1]$, we may use Legendre polynomial $P_N(x)$ of order N. Then any polynomial $f(x)$ of order up to $(2N-1)$ becomes

$$f(x) = Q(x)P_N(x) + R(x) \tag{5.35}$$

with the polynomial $Q(x)$ and $R(x)$ of order up to $(N-1)$. Then the exact integral of $f(x)$ is

$$\int_{-1}^{1} f(x)dx = \int_{-1}^{1} [Q(x)P_N(x) + R(x)]\, dx = \int_{-1}^{1} R(x)dx \tag{5.36}$$

due to the orthogonality of Legendre polynomial Eq.(5.10). If we choose N points x_n to be the N zero points of $P_N(x)$, i.e., $P_N(x_n) = 0$, then the N point numerical integral of $f(x)$, Eq.(5.32) with Eq.(5.35), is

$$\int_{-1}^{1} f(x)dx \approx \sum_{n=1}^{N} w_n [Q(x_n)P_N(x_n) + R(x_n)] = \sum_{n=1}^{N} w_n R(x_n). \tag{5.37}$$

Now we only need to determine the value of N weighting factors w_n which can be done by using Eq.(5.34) with $p = 0, 1, \cdots, (N-1)$. Then

$$w_n = \frac{2}{(1-x_n^2)} \left[\frac{dP_N(x_n)}{dx}\right]^{-2} \tag{5.38}$$

for N points x_n which is the zero point of the Legendre polynomial P_N. This is the Gauss-Legendre quadrature. For $N = 3$,

$$\begin{aligned} x_1 = -x_3 = \sqrt{3/5}, \qquad & x_2 = 0\ ; \\ w_1 = w_3 = 5/9, \qquad & w_2 = 8/9. \end{aligned} \tag{5.39}$$

This 3 point Gauss-Legendre quadrature has the error of order $O(h^7)$ compared to the error of order $O(h^5)$ of the 3 point Simpson's rule. If the integral range is $[a, b] = [0, \infty]$ then we cannot use Gauss-Legendre quadrature. For such a case we may use other orthogonal special function, such as Laguerre polynomial or Hermite polynomial, depending on the form of $f(x)$ instead of Legendre polynomial.