Lecture 4: Series expansions with Special functions

1. Key points

1. Legendre polynomials (Legendre functions)
2. Hermite polynomials (Hermite functions)
3. Laguerre polynomials (Laguerre functions)

Other kinds of special functions such as Bessel functions will be discussed in a later lecture of ordinary differential equations.

Maple commands

LegendreP
HermiteH
LaguerreL

2. Expansion with orthogonal functions

Consider functions \( u_i(x) \), \( i = 1, 2, \cdots, N \) defined in a region \( x \in [a, b] \). They are said to be orthogonal if
\[
\int_a^b w(x) u_i(x) u_j(x) \, dx = \delta_{ij},
\]
where \( w(x) \) is a weight function which depend on the choice of \( u_i(x) \). A function \( f(x) \) defined in the same region can be expressed as a linear combination of \( u_i(x) \):
\[
f(x) = c_1 u_1(x) + c_2 u_2(x) + \cdots = \sum_{i=1}^N c_i u_i(x),
\]
where
\[
c_i = \int_a^b f(x) w(x) u_i(x) \, dx.
\]
and \( N \) is the dimension of the function space. (We will discuss this more in the linear algebra section.)

3. Legendre polynomials

Legendre function \( P_{\ell}(x) \) is a solution to the Legendre differential equation
\[
(1 - x^2) y^{''} - 2 x y^{'} + \ell (\ell + 1) y = 0
\]
\[
(-x^2 + 1) y^{''}(x) - 2 x y^{'}(x) + \ell (\ell + 1) y(x) = 0
\]
When \( \ell \) is 0 or positive integer, \( P_{\ell}(x) \) is a polynomial of order \( \ell \) defined on \( x \in [-1, 1] \).
\[ P_0(x) = \text{simplify}(\text{LegendreP}(0, x)) = 1 \]
\[ P_1(x) = \text{simplify}(\text{LegendreP}(1, x)) = x \]
\[ P_2(x) = \text{simplify}(\text{LegendreP}(2, x)) = -\frac{1}{2} + \frac{3}{2} x^2 \]
\[ P_3(x) = \text{simplify}(\text{LegendreP}(3, x)) = \frac{5}{2} x^3 - \frac{3}{2} x \]

```
plot([[\text{LegendreP}(0, x), \text{LegendreP}(1, x), \text{LegendreP}(2, x), \text{LegendreP}(3, x)], x=-1..1, legend=[
    'P_0(x)', 'P_1(x)', 'P_2(x)', 'P_3(x)']])
```

**Orthogonality**

\[
\int_{-1}^{1} P_{\ell}(x) P_m(x) \, dx = \frac{2}{2\ell + 1} \delta_{\ell m} \\
\int_{-1}^{1} x^m P_{\ell}(x) \, dx = \frac{2 \delta_{\ell m}}{2 \ell + 1}
\]

For \(0 \leq m \leq \ell - 1\), \(\int_{-1}^{1} x^m P_{\ell}(x) \, dx = 0\)
Legendre series

Functions defined on $x \in [-1, 1]$ can be expanded in Legendre series $f(x) = \sum_{\ell=0}^{\infty} c_{\ell} P_{\ell}(x)$

where $c_{\ell} = \frac{2 \ell + 1}{2} \int_{-1}^{1} f(x) P_{\ell}(x) \, dx$

$$c_{\ell} = \frac{(2 \ell + 1)}{2} \left( \int_{-1}^{1} f(x) P_{\ell}(x) \, dx \right)$$

Example

Expand $f(x) = \begin{cases} -1 & -1 < x < 0 \\ 1 & 0 < x < 1 \end{cases}$ in Legendre series.

Using the Heaviside function $\theta(x)$, $f(x) = 2 \theta(x) - 1$, $x \in [-1, 1]$.

Common sense

Heaviside function

$$\theta(x) \equiv \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases}$$

In Maple, the heaviside function is specified as $\text{Heaviside}(x) = \theta(x)$.

Legendre functions of even order have even parity. Since $f(x)$ is an odd function, the coefficients of even order must be zero. Therefore, it is enough to consider only odd order terms.

$$c_{\ell} = \frac{1}{2} (2\ell + 1) \int_{-1}^{1} f(x) P_{\ell}(x) \, dx = (2\ell + 1) \int_{0}^{1} f(x) P_{\ell}(x) \, dx = (2\ell + 1) \int_{0}^{1} P_{\ell}(x) \, dx$$

Common sense

For any even function $f(-x) = f(x)$, $\int_{-a}^{a} f(x) \, dx = 2 \int_{0}^{a} f(x) \, dx$.

For any odd function $f(-x) = -f(x)$, $\int_{-a}^{a} f(x) \, dx = 0$.

for $j$ from 0 to 10 do

$c_{2j+1} := (2 \cdot (2j + 1) + 1) \int_{0}^{1} \text{LegendreP}(2j + 1, x) \, dx$
\begin{align*}
\text{do} \\
\hspace{2cm} c_1 & := \frac{3}{2} \\
\hspace{2cm} c_3 & := -\frac{7}{8} \\
\hspace{2cm} c_5 & := -\frac{11}{16} \\
\hspace{2cm} c_7 & := -\frac{75}{128} \\
\hspace{2cm} c_9 & := \frac{133}{256} \\
\hspace{2cm} c_{11} & := -\frac{483}{1024} \\
\hspace{2cm} c_{13} & := \frac{891}{2048} \\
\hspace{2cm} c_{15} & := -\frac{13299}{32768} \\
\hspace{2cm} c_{17} & := \frac{25025}{65536} \\
\hspace{2cm} c_{19} & := -\frac{94809}{262144} \\
\hspace{2cm} c_{21} & := \frac{180557}{524288}
\end{align*}

unassign('j') : \\
\begin{align*}
h & := x \mapsto \text{sum}(c_{2j + 1} \cdot \text{LegendreP}(2j + 1, x), j = 0..10) \\
h & := x \mapsto \sum_{j=0}^{10} c_{2j + 1} P_{2j + 1}(x)
\end{align*}

\begin{align*}
\text{plot}([2 \cdot \text{Heaviside}(x) - 1, h(x)], x=-1..1, \text{legend}=['f(x)','g(x)'])
\end{align*}
Generating Function

More detailed properties of Legendre polynomials: See [mathworld](http://mathworld.wolfram.com/LegendrePolynomial.html)

**Examples in Physics**

- Dipole moment
Find the potential at position A.

\[
V_1 = \frac{kQ_1}{R} : \\
V_2 = \frac{kQ_2}{d} = \frac{kQ_2}{\sqrt{R^2 - 2Rr \cos(\theta) + r^2}} : 
\]

If \(|r|\) is small enough \(V_2 \approx \frac{kQ_2}{R}\). This equivalent to say that two charges are at the same location. WE want to taken into account the distance \(d\).

\[
V_2 = \frac{kQ_2}{R} \frac{1}{\sqrt{1 - \frac{2r}{R} \cos(\theta) + \left(\frac{r}{R}\right)^2}} : 
\]

Let \(h = \frac{r}{R}\) and \(x = \cos(\theta)\) in the generating function,

\[
V_2 = \frac{kQ_2}{R} \left( P_0(\cos(\theta)) + \frac{r}{R} P_1(\cos(\theta)) + \left(\frac{r}{R}\right)^2 P_2(\cos(\theta)) + \cdots \right) \tag{7}
\]
Coulomb interaction

Consider two charges $Q_1$ and $Q_2$ separated by a distance $d = |\mathbf{r}_1 - \mathbf{r}_2|$. There interaction energy is given by

$$U = \frac{Q_1 Q_2}{|\mathbf{r}_1 - \mathbf{r}_2|}.$$ 

This is mathematically complicated if cartesian coordinates are used. There is a convenient expansion using polar coordinates $|\mathbf{r}_1|$, $|\mathbf{r}_2|$, and angle $\theta$ between $\mathbf{r}_1$ and $\mathbf{r}_2$.

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \frac{1}{r} \sum_{g=0}^{\infty} \left( \frac{r_g}{r} \right)^g P_g(\cos(\theta)),$$

where $r_g = |\mathbf{r}_1|$, $r_s = |\mathbf{r}_2|$ if $|\mathbf{r}_1| > |\mathbf{r}_2|$ and $r_g = |\mathbf{r}_2|$, $r_s = |\mathbf{r}_1|$ if $|\mathbf{r}_1| < |\mathbf{r}_2|$.

\textbf{4. Hermite polynomials}

Hermite polynomials $H_n(x)$, $x \in (-\infty, \infty)$ is a solution to Hermite differential equation

$$y'' - 2x y' + 2ny = 0$$

$$y''(x) - 2x y'(x) + 2ny(x) = 0 \quad (8)$$

When $n$ is 0 or positive integer, $H_n(x)$ are polynomials of order $n$.

$$H_0(x) = \text{simplify}(\text{HermiteH}(0, x)) = 1$$

$$H_1(x) = \text{simplify}(\text{HermiteH}(1, x)) = 2x$$

$$H_2(x) = \text{simplify}(\text{HermiteH}(2, x)) = 4x^2 - 2$$

$$H_3(x) = \text{simplify}(\text{HermiteH}(3, x)) = 8x^3 - 12x$$

plot([\text{HermiteH}(0, x), \text{HermiteH}(1, x), \text{HermiteH}(2, x), \text{HermiteH}(3, x)], x=-1..1, legend=[H_0(x),H_1(x),H_2(x),H_3(x)])}
Orthogonality

\[ \frac{1}{\sqrt{\pi} 2^n n!} \int_{-\infty}^{\infty} e^{-x^2} \frac{H_m(x)}{H_n(x)} \, dx = \delta_{nm}. \]

For \( 0 \leq m \leq n - 1 \), \( \int_{-\infty}^{\infty} x^m H_n(x) \, e^{-x^2} \, dx = 0. \)

Basis functions and weights

There are various ways to define basis functions.

1. \( u_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x), \quad w(x) = e^{-x^2} \)

2. \( u_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x) \, e^{-\frac{x^2}{2}}, \quad w(x) = 1. \)

Which one to use depends on the function to be expanded.
**Hermite series**

Functions defined on \(x \in (-\infty, \infty)\) can be expanded in Hermite series

\[
f(x) = \sum_{n=0}^{\infty} c_n H_n(x).
\]

where

\[
c_n = \frac{1}{2^n n! \sqrt{\pi}} \int_{-\infty}^{\infty} f(x) H_n(x) e^{-x^2} \, dx.
\]

**Example**

Expand \(f(x) = x^8\) in Hermite series.

Since \(\lim_{x \to \pm \infty} f(x) = \infty\) and \(\lim_{x \to \pm \infty} H_n(x) e^{-x^2} = 0\), \(H_n(x) e^{-x^2}\) cannot express \(f(x)\). We use \(H_n(x)\) as basis function.

Since Hermite polynomials of odd order has odd parity, the coefficients of odd order is zero. The terms of order higher than 8 are also all zero. Therefore, we need to consider only five terms (the orders of 0, 2, 4, 6, 8).

\[
f := x \rightarrow x^8;
\]

for \(k\) from 0 by 2 to 10 do

\[
c_k := \frac{1}{2^k k! \sqrt{\pi}} \int_{-\infty}^{\infty} f(x) \text{HermiteH}(k, x) e^{-x^2} \, dx
\]

do

\[
c_0 := \frac{105}{16}
\]

\[
c_2 := \frac{105}{8}
\]

\[
c_4 := \frac{105}{32}
\]

\[
c_6 := \frac{7}{32}
\]

\[
c_8 := \frac{1}{256}
\]

\[
c_{10} := 0
\]

\(\text{unassign}('k'):\)

\(h := x \rightarrow \text{sum}(c_{2k} \text{HermiteH}(2k, x), k = 0..5)\)

\[
h := x \rightarrow \sum_{k=0}^{5} c_{2k} H_{2k}(x)
\]

\(\text{plot}([f(x), h(x)], x=-1..1, \text{legend}=['f(x)', 'h(x)'])\)
This plot shows that the expansion exactly matches to $x^8$.

**Hermite expansion**

For a function $f(x)$, $x \in (-\infty, \infty)$ and $\lim_{|x| \to \infty} f(x) = 0$, the previous expansion does not work since $H_n(x)$ diverges at $|x| \to \infty$. In physics, the following expansion is more popular.

$$f(x) = \sum_{n=0}^{\infty} c_n u_n(x)$$

where

$$u_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x) e^{-\frac{x^2}{2}}.$$

The expansion coefficient can be obtained by

$$c_n = \int_{-\infty}^{\infty} f(x) u_n(x) \, dx$$

Note that $\lim_{|x| \to \infty} u_n(x) = 0$.

**Example**

Expand $e^{-|x|}$ with Hermite polynomials.
Sinf the function is even, the odd terms vanish. Let us calculate the coefficients up to order 10.

\[ f := x \rightarrow e^{-x} : \]

\[ \text{for } k \text{ from 0 to 2 to 10 do } \]
\[ c_k := \frac{2}{\sqrt{2^k k! \sqrt{\pi}}} \int_0^\infty f(x) \cdot \text{HermiteH}(k, x) \cdot e^{-\frac{x^2}{2}} \, dx \]
\[ \text{do } \]
\[ c_0 := \frac{2}{\pi} \left( -\frac{\text{erf}\left(\frac{\sqrt{2}}{2}\right)}{2} \frac{\sqrt{\pi} e^{\frac{1}{2}} \sqrt{2}}{2} + \frac{\sqrt{\pi} e^{\frac{1}{2}} \sqrt{2}}{2} \right) \]
\[ c_2 := \frac{\sqrt{2}}{2 \pi} \left( -4 - 3 \text{erf}\left(\frac{\sqrt{2}}{2}\right) \frac{\sqrt{\pi} e^{\frac{1}{2}} \sqrt{2}}{2} + 3 \sqrt{\pi} e^{\frac{1}{2}} \sqrt{2} \right) \]
\[ c_4 := \frac{\sqrt{6}}{24 \pi} \left( -48 - 38 \text{erf}\left(\frac{\sqrt{2}}{2}\right) \frac{\sqrt{\pi} e^{\frac{1}{2}} \sqrt{2}}{2} + 38 \sqrt{\pi} e^{\frac{1}{2}} \sqrt{2} \right) \]
\[ c_6 := \frac{\sqrt{5}}{240 \pi} \left( -912 - 692 \text{erf}\left(\frac{\sqrt{2}}{2}\right) \frac{\sqrt{\pi} e^{\frac{1}{2}} \sqrt{2}}{2} + 692 \sqrt{\pi} e^{\frac{1}{2}} \sqrt{2} \right) \]
\[ c_8 := \frac{\sqrt{70}}{13440 \pi} \left( -21120 - 16200 \text{erf}\left(\frac{\sqrt{2}}{2}\right) \frac{\sqrt{\pi} e^{\frac{1}{2}} \sqrt{2}}{2} + 16200 \sqrt{\pi} e^{\frac{1}{2}} \sqrt{2} \right) \]
\[ c_{10} := \frac{\sqrt{7}}{80640 \pi} \left( -604992 - 460592 \text{erf}\left(\frac{\sqrt{2}}{2}\right) \frac{\sqrt{\pi} e^{\frac{1}{2}} \sqrt{2}}{2} + 460592 \sqrt{\pi} e^{\frac{1}{2}} \sqrt{2} \right) \]

Here \( \text{erf}() \) is the error function defined by

\[ \text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t} \, dt. \]

The numerical value of the coefficients are:

\[ \text{for } k \text{ from 0 to 2 to 10 do } \]
\[ C_k := \text{evalf}(c_k) \]
\[ \text{do } = \]
\[ C_0 := 0.9849953074 \]
\[ C_2 := -0.03501328428 \]
Now, we have an approximate expression of $f(x)$ using Hermite polynomials.

\[ h := x \rightarrow \text{sum} \left( \frac{1}{\sqrt{2^{2k} (2k)! \sqrt{\pi}}} \text{HermiteH}(2k, x) e^{-\frac{x^2}{2}}, k = 0..5 \right) \]

\[ h := x \mapsto \sum_{k=0}^{5} \frac{C_{2k} H_{2k}(x) e^{-\frac{x^2}{2}}}{\sqrt{2^{2k} (2k)! \sqrt{\pi}}} \]

plot([f(x), h(x)], x = 0..3, legend = ['f(x)', 'h(x)'])
Agreement is not bad. Adding more terms will improve the agreement.

Example in Physics: Quantum Harmonic Oscillator

Schrödinger Equation: \( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m\omega^2}{2} x^2 \psi(x) = E \psi(x) \)

Let \( n = \frac{E}{\hbar\omega} - \frac{1}{2}, \xi = \sqrt{\frac{m\omega}{\hbar}} x \), and \( \psi(x) = e^{-\frac{\xi^2}{2}} u(\xi) \). Then, the Schrödinger equation becomes

\[
\frac{d^2 u}{d\xi^2} - 2\xi \frac{du}{d\xi} + 2nu = 0
\]

which is Hermite equation. Hence,

\[
\psi(x) = C e^{-\frac{m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}} x \right) \text{ and } E = \hbar \omega \left( n + \frac{1}{2} \right) \text{ where } n \in \mathbb{Z}^*.
\]

5. Laguerre polynomials

Laguerre function \( L_n(x), x \in [0, \infty) \) is a solution to the Laguerre differential equation

\[ \frac{x y''}{2} + \frac{(1 - x) y'}{2} + ny = 0. \]

When \( n \) is 0 or a positive integer, \( L_n(x) \) is a polynomial of order \( n \).

\[
L_0(x) = \text{ simplify}(\text{LaguerreL}(0,x)) = 1 \\
L_1(x) = \text{ simplify}(\text{LaguerreL}(1,x)) = 1 - x \\
L_2(x) = \text{ simplify}(\text{LaguerreL}(2,x)) = 1 - 2x + \frac{1}{2}x^2 \\
L_3(x) = \text{ simplify}(\text{LaguerreL}(3,x)) = 1 - 3x + \frac{3}{2}x^2 - \frac{1}{6}x^3
\]

plot([\text{LaguerreL}(0,x), \text{LaguerreL}(1,x), \text{LaguerreL}(2,x), \text{LaguerreL}(3,x)], x = 0 .. 5, legend = ['L_0(x)', 'L_1(x)', 'L_2(x)', 'L_3(x)'])
Orthogonality

\[ \int_0^\infty e^{-x} L_m(x) L_n(x) \, dx = \delta_{mn}, \]

Laguerre series

Functions defined on \( x \in [0, \infty) \) can be expanded in Laguerre series

\[ f(x) = \sum_{n=0}^\infty c_n L_n(x), \]

where \( c_n = \int_0^\infty f(x) L_n(x) e^{-x} \, dx. \)

Exercise
Expand \( f(x) = x^3 e^{-\frac{x}{2}} \) in the Laguerre series. Shows the first 5 terms and compare it with the original function.

\[
f := x \rightarrow x^3 e^{-\frac{x}{2}} : \\
\text{for } k \text{ from 0 to 4 do} \\
c_k := \int_0^\infty f(x) \text{ LaguerreL}(k, x) e^{-x} \, dx \\
\text{do}
\]

\[
c_0 := \frac{32}{27} \\
c_1 := -\frac{160}{81} \\
c_2 := \frac{32}{243} \\
c_3 := \frac{352}{729} \\
c_4 := \frac{544}{2187} \tag{14}
\]

\text{unassign('k') :} \\
h := x \rightarrow \text{sum}(c_k \text{ LaguerreL}(k, x), k = 0 .. 4)

\[
h := x \mapsto \sum_{k=0}^4 c_k L_k(x) \tag{15}
\]

\text{plot([f(x), h(x)], x = 0..2, legend = [f(x)', h(x)'])}
The approximation with the first 5 terms is not so bad.

Homework: Due 9/12, 11am

3.1 Legendre polynomials
Express $3x^2 + x - 1$ as a linear combination of Legendre polynomials.

3.2 Hermite polynomials
Express $2x^3 - x^2 + 1$ as a linear combination of Hermite polynomials.