Chapter 2

Basic Mathematical Operations

2.1 Lagrange n-points Interpolation

For n-points, Lagrange interpolation (내삽법) of function $f(x)$ is

$$f(x) = \sum_{i=1}^{n} \prod_{j \neq i}^{n} \left(\frac{x - x_j}{x_i - x_j} \right) f_i \tag{2.1}$$

where f_i is the value of function $f(x_i)$ at grid point x_i. For 2-points, as a special case,

$$f(x) \approx \frac{x - x_1}{x_0 - x_1} f_0 + \frac{x - x_0}{x_1 - x_0} f_1 = f_0 + \frac{f_1 - f_0}{x_1 - x_0}(x - x_0). \tag{2.2}$$

If we have equally spaced grid points $x_i = ih$ with step size h, the interpolation around $x_0 = 0$ is

$$f(x) = f_0 \pm \frac{f_{\pm 1} - f_0}{h} x \tag{2.3}$$

for 2-points. For 3-points

$$f(x) \approx f_0 + \frac{f_1 - f_{-1}}{2h} x + \frac{f_1 - 2f_0 + f_{-1}}{2h^2} x^2. \tag{2.4}$$

For 4-points

$$\begin{aligned} f(x) &\approx f_0 \pm \frac{1}{6h}(-2f_{\mp 1} - 3f_0 + 6f_{\pm 1} - f_{\pm 2})x + \frac{1}{2h^2}(f_{-1} - 2f_0 + f_1)x^2 \\ &\quad \pm \frac{1}{6h^3}(-f_{\mp 1} + 3f_0 - 3f_{\pm 1} + f_{\pm 2})x^3. \end{aligned} \tag{2.5}$$

For 5 points

$$\begin{aligned} f(x) &= f_0 + \frac{1}{12h}(f_{-2} - 8f_{-1} + 8f_1 - f_2)x \\ &\quad + \frac{1}{24h^2}(-f_{-2} + 16f_{-1} - 30f_0 + 16f_1 - f_2)x^2 \\ &\quad + \frac{1}{12h^3}(-f_{-2} + 2f_{-1} - 2f_1 + f_2)x^3 \\ &\quad + \frac{1}{24h^4}(f_{-2} - 4f_{-1} + 6f_0 - 4f_1 + f_2)x^4. \end{aligned} \tag{2.6}$$

2.2 Numerical Differentiation

Taylor series expansion;

$$f(x) = f_0 + xf' + \frac{x^2}{2!}f'' + \frac{x^3}{3!}f''' + \frac{x^4}{4!}f'''' + \cdots. \tag{2.7}$$

At the discretized grid points,

$$\begin{aligned} f(0) &= f_0, \\ f(\pm h) &= f_{\pm 1} = f_0 \pm hf' + \frac{h^2}{2!}f'' \pm \frac{h^3}{3!}f''' + \frac{h^4}{4!}f'''' + \cdots, \quad (2.8) \\ f(\pm 2h) &= f_{\pm 2} = f_0 \pm 2hf' + \frac{4h^2}{2!}f'' \pm \frac{8h^3}{3!}f''' + \frac{16h^4}{4!}f'''' + \cdots. \end{aligned}$$

Using Eqs.(2.8) or by differentiating the interpolated function of Sect.2.1 we can obtain the numerical differential form of a function.

First order numerical differential form of function $f(x)$ at $x = 0$:
For 2-points (linear);

$$f' \approx \frac{f_1 - f_0}{h} + O(h) = \frac{f_0 - f_{-1}}{h} + O(h). \tag{2.9}$$

For 3-points, from Eq.(2.4) or Eqs.(2.8);

$$
\begin{aligned}
f_1 - f_{-1} &= 2hf' + \frac{h^3}{3} f''' + O(h^5), \\
f' &= \frac{f_1 - f_{-1}}{2h} - \frac{h^2}{6} f''' + O(h^4) \approx \frac{f_1 - f_{-1}}{2h} + O(h^2). \quad (2.10)
\end{aligned}
$$

This 3-point differential looks like 2-point differential with step size $2h$. However 3-point differential form is symmetric around $x = 0$ where we evaluate the differential while 2-point differential form is not. For 4-points;

$$f' = \pm \frac{1}{6h}(-2f_{\mp 1} - 3f_0 + 6f_{\pm 1} - f_{\pm 2}) + O(h^3). \quad (2.11)$$

For 5-points;

$$f' \approx \frac{1}{12h}[f_{-2} - 8f_{-1} + 8f_1 - f_2] + O(h^4). \quad (2.12)$$

2.3 Higher Order Differentiation

No 2-points 2nd order differential.
3-points 2nd order differential, from Eqs.(2.8),

$$
\begin{aligned}
f_1 - 2f_0 + f_{-1} &= h^2 f'' + O(h^4), \\
f'' &= \frac{f_1 - 2f_0 + f_{-1}}{h^2} + O(h^2). \quad (2.13)
\end{aligned}
$$

4-points 2nd order differential

$$f'' = \frac{1}{h^2}(f_{-1} - 2f_0 + f_1) + O(h^3). \quad (2.14)$$

5-points 2nd order differential

$$f'' = \frac{1}{12h^2}(-f_{-2} + 16f_{-1} - 30f_0 + 16f_1 - f_2) + O(h^4). \quad (2.15)$$

No 3-points 3rd order differential.
4-points 3rd order differential

$$f''' \approx \pm \frac{1}{h^3}(-f_{\mp 1} + 3f_0 - 3f_{\pm 1} + f_{\pm 2}). \quad (2.16)$$

5-points 3rd order differential

$$f''' \approx \frac{1}{2h^3}(-f_{-2} + 2f_{-1} - 2f_1 + f_2). \tag{2.17}$$

No 4-points 4th order differential.
5-points 4th order differential

$$f^{(iv)} \approx \frac{1}{h^4}(f_{-2} - 4f_{-1} + 6f_0 - 4f_1 + f_2). \tag{2.18}$$

2.4 Numerical Integral

We can obtain numerical integration form of function $f(x)$ using the interpolation given in Sect.2.1.

Trapezoidal rule : 2-points linear integral
Two trapezoidal integrals for 3-points,

$$\int_{-h}^{h} f(x)dx = \frac{h}{2}(f_{-1} + 2f_0 + f_1) + O(h^3). \tag{2.19}$$

Simpson's rule : 3-points integral (cf. 3-points Lagrange Interpolation)

$$\int_{-h}^{h} f(x)dx = \frac{h}{3}(f_{-1} + 4f_0 + f_1) + O(h^5). \tag{2.20}$$

For $a < x < b$, by Simpson's rule,

$$\int_a^b f(x)dx = \frac{h}{3}[f(a) + 4f(a+h) + 2f(a+2h) + 4f(a+3h) + 2f(a+4h) + \cdots + 2f(b-2h) + 4f(b-h) + f(b)] \tag{2.21}$$

by discretizing into even number of equal segments (grid size) h.

4-points integral : Simpson's 3/8 rule

$$\int_0^{3h} f(x)dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) + O(h^5). \tag{2.22}$$

5-points integral : Bode's rule

$$\int_0^{5h} f(x)dx = \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) + O(h^7). \tag{2.23}$$

Note here that the 3-point integral and the 4-point integral have the same order of error $O(h^5)$ due to the $\pm$ sign of the odd terms in Eq.(2.8). Thus we usually use 3-point Simpson or 5-point Bode's rule which have the midpoint of integral range as one of the grid points.

If function $f(x)$ has both fast varying region and slowly varying region then we can use different grid size for different region. If we can change fast varying function such as $g(x)e^{-x}$ or function with singular points such as $(1-x^2)^{-1/2}$ with singular point $x = \pm 1$ to a smoothly varying function without singular point within the integration region by changing variable then we can use equal grid size with the new variable after changing the function as a function of the new variable.

2.5 Finding Roots; Finding Zero Points

Simple method using half step size. Choose two points x_i and $x_{i+1} = x_i + h$. If

$$f(x_{i+1})f(x_i) > 0, \tag{2.24}$$

then move to next point. If $|f(x_i)| < |f(x_{i+1})|$ then change h to $-h$. If

$$f(x_{i+1})f(x_i) < 0, \tag{2.25}$$

then change h to $h/2$. If this condition is satisfied with $|x_{i+1} - x_i|$ less than allowed error then the zero point is x_i.

Newton-Raphson method. Find the new point x_{i+1} using the differential $f'(x)$ of function $f(x)$.

$$\begin{aligned} f(x_{i+1}) &\approx f(x_i) + (x_{i+1} - x_i)f'(x_i) = 0, \\ x_{i+1} &= x_i - \frac{f(x_i)}{f'(x_i)}. \end{aligned} \tag{2.26}$$

Secant method. Use $f(x_{i-1})$ and $f(x_i)$ for $f'(x_i)$ in Newton-Raphson method.

$$\begin{aligned} f'(x_i) &\approx \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}, \\ x_{i+1} &= x_i - f(x_i)\frac{x_i - x_{i-1}}{f(x_i) - f(x_{i-1})}. \end{aligned} \tag{2.27}$$