1 Basic mathematical operations

1.1 Lagrange n-points Interpolation

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

For 2-points

$$f \approx \frac{x - x_1}{x_0 - x_1} f_0 + \frac{x - x_0}{x_1 - x_0} f_1 = f_0 + \frac{f_1 - f_0}{x_1 - x_0}(x - x_0) = f_0 \pm \frac{f_{\pm 1} - f_0}{h} x \tag{2}$$

For 3-points

$$f \approx f_0 + \frac{f_1 - f_{-1}}{2h} x + \frac{f_1 - 2f_0 + f_{-1}}{2h^2} x^2 \tag{3}$$

For 4-points

$$\begin{aligned} f \approx\ & f_0 \pm \frac{1}{6h}(-2f_{\mp 1} - 3f_0 + 6f_{\pm 1} - f_{\pm 2})x + \frac{1}{2h^2}(f_{-1} - 2f_0 + f_1)x^2 \\ & \pm \frac{1}{6h^3}(-f_{\mp 1} + 3f_0 - 3f_{\pm 1} + f_{\pm 2})x^3 \end{aligned} \tag{4}$$

For 5 points

$$\begin{aligned} f =\ & f_0 + \frac{1}{12h}(f_{-2} - 8f_{-1} + 8f_1 + f_2)x + \frac{1}{24h^2}(-f_{-2} + 16f_{-1} - 30f_0 + 16f_1 - f_2)x^2 \\ & + \frac{1}{12h}(-f_{-2} + 2f_{-1} - 2f_1 + f_2)x^3 + \frac{1}{24h^4}(f_{-2} - 4f_{-1} + 6f_0 - 4f_1 + f_2)x^4 \end{aligned} \tag{5}$$

1.2 Numerical Differentiation

Tayler series expansion;

$$f(x) = f_0 + xf' + \frac{x^2}{2!} f'' + \frac{x^3}{3!} f''' + \frac{x^4}{4!} f'''' + \cdots \tag{6}$$

At the discretized grid points,

$$\begin{aligned} f(0) &= f_0 \\ f(\pm h) &= f_{\pm 1} = f_0 \pm hf' + \frac{h^2}{2!} f'' \pm \frac{h^3}{3!} f''' + \frac{h^4}{4!} f'''' + \cdots \\ f(\pm 2h) &= f_{\pm 2} = f_0 \pm 2hf' + \frac{4h^2}{2!} f'' \pm \frac{8h^3}{3!} f''' + \frac{16h^4}{4!} f'''' + \cdots \end{aligned} \tag{7}$$

Numerical Differentiation:
For 2-points (linear);

$$f' \approx \frac{f_1 - f_0}{h} + O(h) = \frac{f_0 - f_{-1}}{h} + O(h) \tag{8}$$

For 3-points;

$$\begin{aligned} f' &= \frac{f_1 - f_{-1}}{2h} - \frac{h^2}{6} f''' + O(h^4) \approx \frac{f_1 - f_{-1}}{2h} + O(h^2) \\ &: \quad f_1 - f_{-1} = 2hf' + \frac{h^3}{3} f''' + O(h^5) \end{aligned} \tag{9}$$

For 4-points;

$$f' = \pm \frac{1}{6h}(-2f_{\mp 1} - 3f_0 + 6f_{\pm 1} - f_{\pm 2}) + O(h^3) \tag{10}$$

For 5-points;

$$f' \approx \frac{1}{12h}[f_{-2} - 8f_{-1} + 8f_1 - f_2] + O(h^4) \tag{11}$$

1.3 Higher Order Differentiation

No 2-points 2nd order differential.
3-points 2nd order differential

$$\begin{aligned} f'' &= \frac{f_1 - 2f_0 + f_{-1}}{h^2} + O(h^2) \\ &: \quad f_1 - 2f_0 + f_{-1} = h^2 f'' + O(h^4) \end{aligned} \tag{12}$$

4-points 2nd order differential

$$f'' = \frac{1}{h^2}(f_{-1} - 2f_0 + f_1) + O(h^3) \tag{13}$$

5-points 2nd order differential

$$f'' = \frac{1}{12h^2}(-f_{-2} + 16f_{-1} - 30f_0 + 16f_1 - f_2) + O(h^4) \tag{14}$$

No 3-points 3rd order differential.

4-points 3rd order differential

$$f''' \approx \pm\frac{1}{h^3}(-f_{\mp 1} + 3f_0 - 3f_{\pm 1} + f_{\pm 2}) \tag{15}$$

5-points 3rd order differential

$$f''' \approx \frac{1}{2h^3}(-f_{-2} + 2f_{-1} - 2f_1 + f_2) \tag{16}$$

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

$$f^{(iv)} \approx \frac{1}{h^4}(f_{-2} - 4f_{-1} + 6f_0 - 4f_1 + f_2) \tag{17}$$

1.4 Numerical Integral

Trapezoidal rule : two of 2-points integral

$$\int_{-h}^{h} f(x)dx = \frac{h}{2}(f_{-1} + 2f_0 + f_1) + O(h^3) \tag{18}$$

Simpson's rule : 3-points integral

$$\int_{-h}^{h} f(x)dx = \frac{h}{3}(f_{-1} + 4f_0 + f_1) + O(h^5) \tag{19}$$

c.f. 3-points Lagrange Interpolation.
For $a < x < b$, by Simpson's rule,

$$\begin{aligned}\int_a^b f(x)dx = \frac{h}{3}[f(a) + 4f(a+h) + 2f(a+2h) + 4f(a+3h) + 2f(a+4h) \\ + \cdots + 2f(b-2h) + 4f(b-h) + f(b)]\end{aligned} \tag{20}$$

discretizing into even number of equal segments (grid size) h.
4-points integral : Simpson's 3/8 rule

$$\int f(x)dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) + O(h^5) \tag{21}$$

5-points integral : Bode's rule

$$\int f(x)dx = \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) + O(h^7) \tag{22}$$

Change of variable and singular points.

1.5 Finding roots; finding zero points

Simple method using half step size.

$$f(x_{i+1})f(x_i) < \text{ or } > 0 \tag{23}$$

Newton-Raphson method

$$\begin{aligned} f(x_{i+1}) &\approx f(x_i) + (x_{i+1} - x_i)f'(x_i) = 0 \\ x_{i+1} &= x_i - \frac{f(x_i)}{f'(x_i)} \end{aligned} \tag{24}$$

Secant method

$$\begin{aligned} f'(x_i) &\approx \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} \\ x_{i+1} &= x_i - f(x_i)\frac{x_i - x_{i-1}}{f(x_i) - f(x_{i-1})} \end{aligned} \tag{25}$$

2 First order ordinary differential equation

Solve differential equation

$$\frac{dy(x)}{dx} = f(x, y) \tag{26}$$

for function $y(x)$ with initial condition $y(x_0) = y_0$. This can be solved by recursion relation starting from y_0 at x_0.

2.1 Euler's method

Using two point differential form, the recursion relation of Euler's method is

$$y_{n+1} = y_n + hf(x_n, y_n) + O(h^2) \tag{27}$$

Since $y' = f(x, y(x))$, we have

$$y'' = \frac{d}{dx}f(x, y) = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}f \tag{28}$$

Thus from Tayler expansion

$$y_{n+1} = y_n + hy'_n + \frac{h^2}{2}y''_n + \frac{h^3}{3!}y'''_n + \cdots \tag{29}$$

we can get higher order recursion relation

$$y_{n+1} = y_n + hf_n + \frac{h^2}{2}\left[\frac{\partial f}{\partial x} + f\frac{\partial f}{\partial y}\right]_n + O(h^3) \tag{30}$$

2.2 Using Extrapolation

Implicit methods using integral of f,

$$y_{n+1} = y_n + \int_{x_n}^{x_{n+1}} f(x,y)dx \tag{31}$$

Use extrapolation or interpolation for $f(x,y)$ here.
Using two points extrapolation, we get Adams-Bashforth 2-step Method

$$y_{n+1} = y_n + \frac{h}{2}(3f_n - f_{n-1}) + O(h^3) \tag{32}$$

Multistep method using multi-points extrapolation.

2.3 Using Interpolation

Adams-Moulton Method
Predictor-Corrector Algorithm

2.4 Runge-Kutta Methods

Use three points Simpson rule for the integral of $f(x,y)$ from y_n to y_{n+1} with three points interpolation of x_n, $x_{n+1/2}$, and x_{n+1}.

$$\begin{aligned} y_{n+1} &= y_n + \int_{y_n}^{y_{n+1}} f(x,y)dx \\ &\approx y_n + \frac{h}{6}\Big[f(x_n,y_n) + 4f(x_{n+1/2},y_{n+1/2}) + f(x_{n+1},y_{n+1})\Big] + \mathcal{O}(h^5) \end{aligned} \tag{33}$$

Three point third order Runge-Kutta method;

$$\begin{aligned} k_1 &= hf(x_n,y_n) \\ k_2 &= hf(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1) \\ k_3 &= hf(x_n + h, y_n - k_1 + 2k_2) \\ y_{n+1} &= y_n + \frac{1}{6}(k_1 + 4k_2 + k_3) + \mathcal{O}(h^4) \end{aligned} \tag{34}$$

Three point fourth order Runge-Kutta method;

$$\begin{aligned}
k_1 &= hf(x_n, y_n) \\
k_2 &= hf(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1) \\
k_3 &= hf(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_2) \\
k_4 &= hf(x_n + h, y_n + k_3) \\
y_{n+1} &= y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k4) + \mathcal{O}(h^5) \qquad (35)
\end{aligned}$$

2.5 Stability

3 Boundary value and Eigenvalue Problems

Solve second order linear differential equation

$$\frac{d^2y(x)}{dx^2} + k^2(x)y(x) = S(x) \qquad (36)$$

for function $y(x)$.

3.1 Numerov algorithm

$$\begin{aligned}
\left(1 + \frac{h^2}{12}k_{n+1}^2\right) y_{n+1} &- 2\left(1 - 5\frac{h^2}{12}k_n^2\right) y_n + \left(1 + \frac{h^2}{12}k_{n-1}^2\right) y_{n-1} \qquad (37) \\
&= \frac{h^2}{12}\left(S_{n+1} + 10S_n + S_{n-1}\right) + \mathcal{O}(h^6) \qquad (38)
\end{aligned}$$