Numerical Modeling

Unit 3:Numerical Differentiation and Integration

Numerical Differentiation

- A1. Numerical Differentiation

  - for a function/data set $f(x)$ we define the derivative in a point x_0 as:

$$f'(x_n) = \frac{df}{dx}(x_n) = \lim_{x \to x_n} \frac{f(x) - f(x_n)}{x - x_n}$$

  - using Taylor expansion form we can express

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k + E(x - x_0)^{n+1}$$

- One note ...

Numerical Differentiation

- A1. Numerical Differentiation

  - forward difference

$$f(x_{n+1}) = f(x_n) + f'(x_n)(x_{n+1} - x_n) + f''(x_n)\frac{(x_{n+1} - x_n)^2}{2!} + E(x_{n+1} - x_n)^3$$

$$f'(x_n) = \frac{f(x_{n+1}) - f(x_n)}{x_{n+1} - x_n} + O(x_{n+1} - x_n)$$

  - backward difference

$$f(x_{n-1}) = f(x_n) + f'(x_n)(x_{n-1} - x_n) + f''(x_n)\frac{(x_{n-1} - x_n)^2}{2!} + E(x_{n-1} - x_n)^3$$

$$f'(x_n) = \frac{f(x_{n-1}) - f(x_n)}{x_{n-1} - x_n} + O(x_{n-1} - x_n)$$

  - central difference

1

$$f'(x_n) = \frac{f(x_{n+1}) - f(x_{n-1})}{x_{n+1} - x_{n-1}} + O(x_{n+1} - x_{n\cancel{-1}})^2$$

- One note

Numerical Differentiation

- A2. Numerical Differentiation – 3-point formula

\- for $f'(x)$ by using Lagrange extension

2

$$f'(x_n) = \frac{1}{2h}[-3f(x_n) + 4f(x_{n+1}) - f(x_{n+2})] + E(h^2)$$

$$f'(x_n) = \frac{1}{2h}[-f(x_{n-1}) + f(x_{n+1})] + E(h^2)$$

Numerical Differentiation

- A2. Numerical Differentiation 2nd degree

  - using Taylor expansion

3

$$f''(x_n) = \frac{1}{h^2}[f(x_{n-1}) - 2f(x_n) + f(x_{n+1})] + E(h^2)$$

- One note ...

Numerical Integration

- B2. Implementations

Midpoint Implementation

$$\int_a^b f(x)dx = hf(\frac{a+b}{2}) + O(h^3)$$

Trapezoidal Implementation

4

$$\int_a^b f(x)dx = h\frac{f(a)+f(b)}{2} + O(h^3)$$

Simpson Implementation (from 2nd degree polynomial aproximation)

$$\int_{x_0}^{x_2} f(x)dx = h\frac{f(x_0)+4f(x_1)+f(x_2)}{3} + O(h^5)$$

Numerical Integration

- B1. Definitions

$$\int f(x)dx = \lim_{n\to\infty} \sum_{i=1}^{n} f(x_i)dx$$

$$\iint f(x,y)ds = \lim_{m,n\to\infty} \sum_{i=1}^{n} \sum_{j=1}^{m} f(x_i, y_j)ds$$

5

$$\int_a^b \int_m^n f(x,y)\,dx\,dy \cong \sum_{i=1}^{steps\_x} \sum_{j=1}^{steps\_y} h\cdot k\cdot f(a+i\cdot h,\ m+j\cdot k)$$