Numerical Analysis
Numerical Differentiation

목 차

Finite Difference Formula using Taylor Series Expansion

Lecture Note-Numerical Analysis: Numerical differentiation

1. Taylor Series Expansion and Function Derivatives Revisited

- Taylor series expansion of f(x+h) for a small value h around a given point x

$$f(x+h) \approx f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{6}f^{(3)}(x)h^3 + O(h^4)$$

$$f(x-h) \approx f(x) - f'(x)h + \frac{1}{2}f''(x)h^2 - \frac{1}{6}f^{(3)}(x)h^3 + O(h^4)$$

$$f(x+2h) \approx f(x) + 2f'(x)h + 2f''(x)h^2 + \frac{4}{3}f^{(3)}(x)h^3 + O(h^4)$$

$$f(x-2h) \approx f(x) - 2f'(x)h + 2f''(x)h^2 + \frac{3}{4}f^{(3)}(x)h^3 + O(h^4)$$

$$\vdots$$

- The 1st order approximation of the 1st derivative of f(x) using one of the above equation

$$f'(x) \approx \frac{1}{h}\{f(x+h) - f(x)\} + \frac{1}{2}f''(x)h + \frac{1}{6}f^{(3)}(x)h^2 + O(h^3) \approx \frac{1}{h}\{f(x+h) - f(x)\} + O(h)$$

or

$$f'(x) \approx \frac{1}{h}\{f(x) - f(x-h)\} + \frac{1}{2}f''(x)h - \frac{1}{6}f^{(3)}(x)h^2 + O(h^3) \approx \frac{1}{h}\{f(x+h) - f(x)\} + O(h)$$

Therefore, the first order numerical approximation becomes

Forward difference formula (1st order) $\boxed{f'(x) \approx \frac{1}{h}\{f(x+h) - f(x)\}}$

Backward difference formula (1st order) $\boxed{f'(x) \approx \frac{1}{h}\{f(x) - f(x-h)\}}$

Finite Difference Formula using Taylor Series Expansion

- The 2nd order approximation of the 1st derivative of f(x) by subtracting the above equation

$$f(x+h)-f(x-h)\approx 2f'(x)h+\frac{2}{6}f^{(3)}(x)h^3+O(h^4)$$

$$f'(x)\approx\frac{1}{2h}\{f(x+h)-f(x-h)\}-\frac{1}{6}f^{(3)}(x)h^2+O(h^3)\approx\frac{1}{2h}\{f(x+h)-f(x-h)\}+O(h^2)$$

Therefore, the 2nd order numerical approximation becomes

Central difference formula (2nd order)

$$\boxed{f'(x)\approx\frac{1}{2h}\{f(x+h)-f(x-h)\}}$$

- **2nd derivative (2nd order)**

Using

$$f(x+h)\approx f(x)+f'(x)h+\frac{1}{2}f''(x)h^2+\frac{1}{6}f^{(3)}(x)h^3+O(h^4)$$

$$f(x-h)\approx f(x)-f'(x)h+\frac{1}{2}f''(x)h^2-\frac{1}{6}f^{(3)}(x)h^3+O(h^4)$$

Adding two equations,

$$f(x+h)+f(x-h)\approx 2f(x)+f''(x)h^2+\frac{1}{3}f^{(3)}(x)h^3+O(h^4)$$

$$\rightarrow \boxed{f''(x)=\frac{f(x+h)-2f(x-h)+f(x-h)}{2h^2}+O(h^2)}$$

Finite Difference Formula using Taylor Series Expansion

2. Higher Order Derivatives at equally spaced nodes

- High-accuracy divided-difference formulas can be generated by including additional terms from the Taylor series expansion.

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(x_i)}{2}h + O(h^2)$$

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h)$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{2h^2}h + O(h^2)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2)$$

- Inclusion of the 2nd derivative term has improved the accuracy to $O(h^2)$.
- Similar improved versions can be developed for the backward and centered formulas as well as for the approximations of the higher derivatives.

Finite Difference Formula using Newton Interpolation

3. Higher Order Function Derivatives at unequally spaced nodes

- Using the divided difference interpolating polynomial

$$\boxed{\begin{aligned}
f(x) &= b_0 + b_1(x-x_0) + b_2(x-x_0)(x-x_1) + \cdots + b_{n-1}(x-x_0)(x-x_1)\cdots(x-x_{n-1}) \\
&\quad + b_n(x-x_0)(x-x_1)\cdots(x-x_{n-1})(x-x_n) \\[1em]
b_0 &= f[x_0] \\
b_1 &= f[x_1, x_0] \\
b_2 &= f[x_2, x_1, x_0] \\
&\vdots \\
b_{n-2} &= f[x_{n-2} \cdots, x_2, x_1, x_0] \\
b_{n-1} &= f[x_{n-1}, x_{n-2} \cdots, x_2, x_1, x_0] \\
b_n &= f[x_n, x_{n-1}, x_{n-2} \cdots, x_2, x_1, x_0]
\end{aligned}}$$

0^{th} order: $\boxed{f[x_i] = f(x_i)}$

1^{st} order: $\boxed{f[x_i, x_j] = \dfrac{f[x_i] - f[x_j]}{(x_i - x_j)}}$

2^{nd} order: $\boxed{f[x_i, x_j, x_k] = \dfrac{f[x_i, x_j] - f[x_j, x_k]}{(x_i - x_k)}}$

…….

n^{th} order: $\boxed{f[x_n, x_{n-1}, x_{n-1}, \cdots, x_1, x_0] = \dfrac{f[x_n, x_{n-1}, x_{n-2}, \cdots, x_1] - f[x_{n-1}, x_{n-2}, \cdots, x_1, x_0]}{(x_n - x_0)}}$

Finite Difference Formula using Newton Interpolation

- 1^{st} derivatives

$$f'(x) = b_1 + b_2\{(x-x_0)+(x-x_1)\} + b_3\{(x-x_1)(x-x_2)+(x-x_0)(x-x_2)+(x-x_0)(x-x_1)\} + \cdots$$

At $x = x_0$,

$$f'(x_0) = b_1 + b_2\{(x_0-x_1)\} + b_3\{(x_0-x_1)(x_0-x_2)\} + b_4\{(x_0-x_1)(x_0-x_2)(x_0-x_3)\}\cdots$$
$$= b_1 + O(h) \rightarrow \text{forward difference}$$
$$= b_1 + b_2\{(x_0-x_1)\} + O(h^2) \rightarrow \text{forward difference}$$
$$= b_1 + b_2\{(x_0-x_1)\} + b_3\{(x_0-x_1)(x_0-x_2)\} + O(h^3)$$

At $x = x_1$,

$$f'(x_1) = b_1 + b_2\{(x_1-x_0)\} + b_3\{(x_1-x_0)(x_1-x_2)\} + b_4\{(x_1-x_0)(x_1-x_2)(x_1-x_3)\}\cdots$$
$$= b_1 + O(h) \rightarrow \text{backward difference}$$
$$= b_1 + b_2\{(x_1-x_0)\} + O(h^2) \rightarrow \text{central difference}$$
$$= b_1 + b_2\{(x_1-x_0)\} + b_3\{(x_1-x_0)(x_1-x_2))\} + O(h^3)$$

- 2^{nd} derivatives

$$f''(x) = 2b_2 + 2b_3\{(x-x_0)+(x-x_1)+(x-x_2)\} + \cdots$$

- Etc

→ **<u>If we apply the equal spacing condition to above relations, the higher order function derivatives can be obtained for equally spaced data</u>**

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End of Lecture