Advanced Methods on Computational Physics

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Exercise Set 8

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Run the programs with main.sh bash file.

1.

According to Teylor series for each point we have

$$f(x+\Delta x) = f(x) + \Delta x f'(x) + \frac{\Delta x^2}{2!} f''(x) + \frac{\Delta x^3}{3!} f'''(x) + \frac{\Delta x^4}{4!} f^{(4)}(x) + \frac{\Delta x^5}{5!} f^{(5)}(x) + \frac{\Delta x^6}{6!} f^{(6)}(x) + \frac{\Delta x^7}{7!} f^{(7)}(x) + \cdots$$

$$f(x-\Delta x) = f(x) - \Delta x f'(x) + \frac{\Delta x^2}{2!} f''(x) - \frac{\Delta x^3}{3!} f'''(x) + \frac{\Delta x^4}{4!} f^{(4)}(x) - \frac{\Delta x^5}{5!} f^{(5)}(x) + \frac{\Delta x^6}{6!} f^{(6)}(x) - \frac{\Delta x^7}{7!} f^{(7)}(x) + \cdots$$

$$f(x+2\Delta x) = f(x) + 2\,\Delta x f'(x) + \frac{4\Delta x^2}{2!} f''(x) + \frac{8\Delta x^3}{3!} f'''(x) + \frac{16\Delta x^4}{4!} f^{(4)}(x) + \frac{32\Delta x^5}{5!} f^{(5)}(x) + \frac{64\Delta x^6}{6!} f^{(6)}(x) + \frac{128\Delta x^7}{7!} f^{(7)}(x) + \cdots$$

$$f(x-2\Delta x) = f(x) - 2\,\Delta x f'(x) + \frac{4\Delta x^2}{2!} f''(x) - \frac{8\Delta x^3}{3!} f'''(x) + \frac{16\Delta x^4}{4!} f^{(4)}(x) - \frac{32\Delta x^5}{5!} f^{(5)}(x) + \frac{64\Delta x^6}{6!} f^{(6)}(x) - \frac{128\Delta x^7}{7!} f^{(7)}(x) + \cdots$$

$$f(x+3\Delta x) = f(x) + 3\,\Delta x f'(x) + \frac{9\Delta x^2}{2!} f''(x) + \frac{27\Delta x^3}{3!} f'''(x) + \frac{81\Delta x^4}{4!} f^{(4)}(x) + \frac{243\Delta x^5}{5!} f^{(5)}(x) + \frac{729\Delta x^6}{6!} f^{(6)}(x) + \frac{2187\Delta x^7}{7!} f^{(7)}(x) + \cdots$$

$$f(x-3\Delta x) = f(x) - 3\,\Delta x f'(x) + \frac{9\Delta x^2}{2!} f''(x) - \frac{27\Delta x^3}{3!} f'''(x) + \frac{81\Delta x^4}{4!} f^{(4)}(x) - \frac{243\Delta x^5}{5!} f^{(5)}(x) + \frac{729\Delta x^6}{6!} f^{(6)}(x) - \frac{2187\Delta x^7}{7!} f^{(7)}(x) + \cdots$$

$$f(x+4\Delta x) = f(x) + 4\Delta x f'(x) + \frac{16\Delta x^2}{2!} f''(x) + \frac{64\Delta x^3}{3!} f'''(x) + \frac{256\Delta x^4}{4!} f^{(4)}(x) + \frac{1024\Delta x^5}{5!} f^{(5)}(x) + \frac{4096\Delta x^6}{6!} f^{(6)}(x) + \frac{16384\Delta x^7}{7!} f^{(7)}(x) + \cdots$$

$$f(x-4\Delta x) = f(x) - 4\Delta x f'(x) + \frac{16\Delta x^2}{2!} f''(x) - \frac{64\Delta x^3}{3!} f'''(x) + \frac{256\Delta x^4}{4!} f^{(4)}(x) - \frac{1024\Delta x^5}{5!} f^{(5)}(x) + \frac{4096\Delta x^6}{6!} f^{(6)}(x) - \frac{16384\Delta x^7}{7!} f^{(7)}(x) + \cdots$$

The even powers will simplify by subtracting symmetrical points and for odd powers we should find the appropriate coefficients

7-Point CD

$$45 \times [f(x+\Delta x) - f(x-\Delta x) = 2\Delta x f'(x) + \frac{2\Delta x^3}{3!} f'''(x) + \frac{2\Delta x^5}{5!} f^{(5)}(x) + O(\Delta x^6)]$$

$$-9 \times [f(x+2\Delta x) - f(x-2\Delta x) = 4\,\Delta x f'(x) + \frac{16\Delta x^3}{3!} f'''(x) + \frac{64\Delta x^5}{5!} f^{(5)}(x) + O(\Delta x^6)]$$

$$f(x+3\Delta x) - f(x-3\Delta x) = 6\,\Delta x f'(x) + \frac{54\Delta x^3}{3!} f'''(x) + \frac{486\Delta x^5}{5!} f^{(5)}(x) + O(\Delta x^6)$$

$$\Rightarrow$$

$$\boxed{f'(x) = \frac{-f(x-3\Delta x) + 9f(x-2\Delta x) - 45f(x-\Delta x) + 45f(x+\Delta x) - 9f(x+2\Delta x) + f(x+3\Delta x)}{60\Delta x}}$$

9-Point CD

$$672 \times [f(x+\Delta x) - f(x-\Delta x) = 2\Delta x f'(x) + \frac{2\Delta x^3}{3!} f'''(x) + \frac{2\Delta x^5}{5!} f^{(5)}(x) + 2\Delta x^7 f^{(7)}(x) + O(\Delta x^8)]$$

$$-168 \times [f(x+2\Delta x) - f(x-2\Delta x) = 4\,\Delta x f'(x) + \frac{16\Delta x^3}{3!} f'''(x) + \frac{64\Delta x^5}{5!} f^{(5)}(x) + \frac{256\Delta x^7}{7!} f^{(7)}(x) + O(\Delta x^8)]$$

$$32 \times [f(x+3\Delta x) - f(x-3\Delta x) = 6\,\Delta x f'(x) + \frac{54\Delta x^3}{3!} f'''(x) + \frac{486\Delta x^5}{5!} f^{(5)}(x) + \frac{1458\Delta x^7}{7!} f^{(7)}(x) + O(\Delta x^8)]$$

$$-3 \times [f(x+4\Delta x) - f(x-4\Delta x) = 8\,\Delta x f'(x) + \frac{128\Delta x^3}{3!} f'''(x) + \frac{2048\Delta x^5}{5!} f^{(5)}(x) + \frac{32768\Delta x^7}{7!} f^{(7)}(x) + O(\Delta x^8)]$$

$$\Rightarrow$$

$$\boxed{\begin{aligned} f'(x) = \{&3f(x-4\Delta x) - 32f(x-3\Delta x) + 168f(x-2\Delta x) - 672f(x-\Delta x) + 672f(x+\Delta x) \\ &- 168f(x+2\Delta x) + 32f(x+3\Delta x) - 3f(x+4\Delta x)\}/(840\Delta x)\end{aligned}}$$

2. For implicit method we have

$$f(x+\Delta x) = f(x) + \Delta x f'(x+\Delta x)$$

A:

$$f'(x) = f^2(x)$$

$$f(x+\Delta x) = f(x) + \Delta x f^2(x+\Delta x) \rightarrow$$

$$\Delta x f^2(x+\Delta x) - f(x+\Delta x) + f(x) = 0 \rightarrow$$

$$f(x+\Delta x) = \frac{1 \pm \sqrt{1 - 4\Delta x f(x)}}{2\Delta x}$$

B:

$$f'(x) = -f(x)$$

$$f(x+\Delta x) = f(x) - \Delta x f(x+\Delta x) \rightarrow$$

$$f(x+\Delta x) = \frac{f(x)}{1+\Delta x}$$