Homework 1: Report

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Problem 1:

1. Derive the four-point finite-difference backward differentiation formula (BDF3) ap- proximation of the first derivative of f.

   Proof.

$$f'(x_j) \simeq \frac{11f(x_j) - 18f(x_{j-1}) + 9f(x_{j-2}) - 2f(x_{j-3})}{6\Delta x} \tag{1}$$

We start with the polynomial approximation $f(x) \simeq \prod_4 f(x)$ as a 4 point polynomial interpolation with lagranian polynomials. Also note that I will be using the notation of $x_0 = x_{j-3}$, $x_1 = x_{j-2}$, $x_2 = x_{j-1}$, $x_3 = x_j$.

$$f(x) \simeq \prod_4 f(x) = f(x_0)l_0(x) + f(x_1)l_1(x) + f(x_2)l_2(x) + f(x_3)l_3(x) \tag{2}$$

$$\frac{df}{dx} \simeq \frac{d\prod_4 f}{dx} = f(x_0)l_0'(x) + f(x_1)l_1'(x) + f(x_2)l_2'(x) + f(x_3)l_3'(x) \tag{3}$$

We will now look at $f'(x_3) \simeq \frac{d\prod_4 f}{dx}(x_3)$. To reduce its complexity we look at the individual components $l_i'(x_3)$ first. For $i \neq 3$ we have,

$$l_i'(x) = \left(\prod_{j\neq i} \frac{1}{x_i - x_j}\right) \frac{d\prod_{j\neq i}(x - x_j)}{dx} \tag{4}$$

$$l_i'(x) = \left(\prod_{j\neq i} \frac{1}{x_i - x_j}\right) \sum_{j\neq i} \prod_{k\neq i,j} (x - x_k) \tag{5}$$

$$i \neq 3, \quad l_i'(x_3) = \left(\prod_{j\neq i} \frac{1}{x_i - x_j}\right) \prod_{k\neq i,3} (x_3 - x_k) \tag{6}$$

$$i = 3, \quad l_i'(x_3), = \sum_{j\neq 3} \frac{1}{x_3 - x_j} \tag{7}$$

Finally we assume an evenly spaced grid. That is, $x_3 = x_0 + 3\Delta x$, $x_3 = x_1 + 2\Delta x$, and $x_3 = x_2 + \Delta x$.

$$l_0'(x_3) = \frac{(2\Delta x)(\Delta x)}{(-3\Delta x)(-2\Delta x)(-\Delta x)} = -\frac{1}{3\Delta x} \quad (8)$$

$$l_1'(x_3) = \frac{(3\Delta x)(\Delta x)}{(\Delta x)(-2\Delta x)(-\Delta x)} = \frac{3}{2\Delta x} \quad (9)$$

$$l_2'(x_3) = \frac{(3\Delta x)(2\Delta x)}{(\Delta x)(2\Delta x)(-\Delta x)} = -\frac{3}{\Delta x} \quad (10)$$

$$l_3'(x_3) = \left(\frac{1}{3\Delta x} + \frac{1}{2\Delta x} + \frac{1}{\Delta x}\right) = \frac{11}{6\Delta x} \quad (11)$$

$$f'(x_3) \simeq f(x_0)l_0'(x_3) + f(x_1)l_1'(x_3) + f(x_2)l_2'(x_3) + f(x_3)l_3'(x_3) \quad (12)$$

$$\simeq -\frac{f(x_0)}{3\Delta x} + \frac{3f(x_1)}{2\Delta x} - \frac{3f(x_2)}{\Delta x} + \frac{11f(x_3)}{6\Delta x} \quad (13)$$

$$\simeq \frac{11f(x_3) - 18f(x_2) + 9f(x_1) - 2f(x_0)}{6\Delta x} \quad (14)$$

□

2. Prove that (1) converges with order 3 in Δx to the analytical derivative $f'(x_j)$.

Proof. We begin this proof using taylor polynomial approximations for $f(x)$ centered at x_3 (Note: *h.o.t.* indicates "higher order terms").

$$f(x_2) \simeq f(x_3) - f'(x_3)\Delta x + \frac{f''(x_3)\Delta x^2}{2} - \frac{f'''(x_3)\Delta x^3}{6} + \frac{f''''(x_3)\Delta x^4}{24} + h.o.t. \quad (15)$$

$$f(x_1) \simeq f(x_3) - 2f'(x_3)\Delta x + \frac{4f''(x_3)\Delta x^2}{2} - \frac{8f'''(x_3)\Delta x^3}{6} + \frac{16f''''(x_3)\Delta x^4}{24} + h.o.t. \quad (16)$$

$$f(x_0) \simeq f(x_3) - 3f'(x_3)\Delta x + \frac{9f''(x_3)\Delta x^2}{2} - \frac{27f'''(x_3)\Delta x^3}{6} + \frac{81f''''(x_3)\Delta x^4}{24} + h.o.t. \quad (17)$$

$$\frac{f(x_2) - f(x_3)}{\Delta x} + f'(x_3) \simeq \frac{f''(x_3)\Delta x}{2} - \frac{f'''(x_3)\Delta x^2}{6} + \frac{f''''(x_3)\Delta x^3}{24} + h.o.t. \quad (18)$$

$$\frac{f(x_1) - f(x_3)}{2\Delta x} + f'(x_3) \simeq \frac{2f''(x_3)\Delta x}{2} - \frac{4f'''(x_3)\Delta x^2}{6} + \frac{8f''''(x_3)\Delta x^3}{24} + h.o.t. \quad (19)$$

$$\frac{f(x_0) - f(x_3)}{3\Delta x} + f'(x_3) \simeq \frac{3f''(x_3)\Delta x}{2} - \frac{9f'''(x_3)\Delta x^2}{6} + \frac{27f''''(x_3)\Delta x^3}{24} + h.o.t. \quad (20)$$

Notice that we have 3 equations, and wish to eliminate all terms with second and third derivatives. We now use some basic linear algebra in order to eliminate the desired terms. We will express the desired equation as $A(18) + B(19) + C(20)$, where A, B, C are scalar multipliers. The resulting system of equations is,

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \\ 1 & 4 & 9 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad (21)$$

This system has solution, $A = 3$, $B = -3$, $C = 1$. We obtain a new equation using these scalar coefficients.

$$3\frac{f(x_2) - f(x_3)}{\Delta x} - 3\frac{f(x_1) - f(x_3)}{2\Delta x} + \frac{f(x_0) - f(x_3)}{3\Delta x} + f'(x_3) \simeq f''''(x_3)\Delta x^3 \left(\frac{3}{24} - \frac{24}{24} + \frac{27}{24}\right) + h.o.t. \quad (22)$$

$$\frac{18f(x_2) - 18f(x_3) - 9f(x_1) + 9f(x_3) + 2f(x_0) - 2f(x_3)}{6\Delta x} + f'(x_3) \simeq \frac{f''''(x_3)\Delta x^3}{4} + h.o.t. \tag{23}$$

$$f'(x_3) - \frac{11f(x_3) - 18f(x_2) + 9f(x_1) - 2f(x_0)}{6\Delta x} \simeq \frac{f''''(x_3)\Delta x^3}{4} + h.o.t. \tag{24}$$

$$\left\| f'(x_3) - \frac{11f(x_3) - 18f(x_2) + 9f(x_1) - 2f(x_0)}{6\Delta x} \right\|_\infty \simeq \left\| \frac{f''''(x_3)\Delta x^3}{4} \right\|_\infty = O(\Delta x^3) \tag{25}$$

Thus, this derivative approximation converges cubically with Δx.

□

3. Show numerically that (1) converges with order 3 by applying it to the periodic function,

$$f(x) = \log(2 + \sin(2\pi x))$$

Proof. We first look at the analytical derivative.

$$f'(x) = \frac{1}{\ln(10)(2 + \sin(2\pi x))}(2\pi \cos(2\pi x))$$

Next we implement a scheme in fortran to compute the BDF3 derivative approximation at each step.

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Problem 2: