

In the following examples, we will adopt the notation in the textbook. The unit grid size (" Δx " in our lecture) is denoted as h . It is also understood that, for a uniform grid, $f(x) \rightarrow f(x_i)$, $f(x+h) \rightarrow f(x_{i+1})$, $f(x-h) \rightarrow f(x_{i-1})$, and so on. (The first two examples are relevant to Prob 2 and 3 in our HW4.)

Example 1. (Prob 6.6 in textbook)

Derive a **three-point finite difference formula** for the **second derivative**, $f''(x_i)$, using the three grid points at $x = x_{i-1}$, x_i , and x_{i+1} . The grid is non-uniform with $x_{i+1} - x_i = 2h$ and $x_i - x_{i-1} = h$. See p. 273 in textbook for illustration.

Solution:

Consider the Taylor series expansion at $x = x_{i+1}$ and $x = x_{i-1}$,

$$f(x_{i+1}) = f(x_i) + 2 f'(x_i) h + 2 f''(x_i) h^2 + (4/3) f'''(x_i) h^3 + (2/3) f''''(x_i) h^4 + \dots \quad (\text{I})$$

$$f(x_{i-1}) = f(x_i) - f'(x_i) h + f''(x_i) h^2/2 - f'''(x_i) h^3/6 + f''''(x_i) h^4/24 - \dots \quad (\text{II})$$

Since we have only two Taylor series to manipulate, we have to use them to eliminate the terms with $f'(x_i)$ in order to obtain a scheme for $f''(x_i)$. [We can foresee that the resulted finite difference formula will be of $O(h)$ accuracy only. To obtain a formula with a higher order accuracy, more grid points will have to be used.] To proceed, we simply consider $1 \times (\text{I}) + 2 \times (\text{II})$ which leads to

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

Dividing the above formula by $4 h^2$ leads to the final answer,

$$f''(x_i) = (2f(x_{i-1}) - 3 f(x_i) + f(x_{i+1})) / 3h^2 + O(h) .$$

Example 2.

Derive a **four-point finite difference scheme** with $O(h^3)$ accuracy for the **first derivative** that expresses $f'(x_i)$ as a combination of $f(x_{i-1})$, $f(x_i)$, $f(x_{i+1})$, and $f(x_{i+2})$.

Solution:

Consider the Taylor series expansion at $x = x_{i+1}$, x_{i+2} , and x_{i-1} ,

$$f(x_{i+1}) = f(x_i) + f'(x_i) h + f''(x_i) \frac{h^2}{2} + f'''(x_i) \frac{h^3}{6} + f^{(4)}(x_i) \frac{h^4}{24} + f^{(5)}(x_i) \frac{h^5}{120} + \dots \quad (1)$$

$$f(x_{i+2}) = f(x_i) + 2 f'(x_i) h + 2 f''(x_i) \frac{h^2}{2} + \frac{4}{3} f'''(x_i) \frac{h^3}{6} + \frac{2}{3} f^{(4)}(x_i) \frac{h^4}{24} + \frac{8}{15} f^{(5)}(x_i) \frac{h^5}{120} + \dots \quad (2)$$

$$f(x_{i-1}) = f(x_i) - f'(x_i) h + f''(x_i) \frac{h^2}{2} - f'''(x_i) \frac{h^3}{6} + f^{(4)}(x_i) \frac{h^4}{24} - f^{(5)}(x_i) \frac{h^5}{120} + \dots \quad (3)$$

Our goal is to combine formula (1)-(3) to eliminate all terms that involve $f''(x_i)$, and $f'''(x_i)$ (marked by blue). This will lead to an expression of $f'(x_i) h$ in terms of $f(x)$ at various grid points, and $f^{(4)}(x_i) h^4$ plus higher order terms. Dividing that expression by h should lead to our final formula with $O(h^3)$ discretization error. To proceed, we can assume that the final formula is a linear combination of (1)-(3),

$$A \times (1) + B \times (2) + C \times (3) ,$$

and solve the ratio of $A : B : C$ (we can only solve for the ratios because there will be only two equations for three unknowns). Since the finite difference formula is not affected by multiplication or division by a constant, we can divide the above expression by A to obtain a simpler formula (we have cleaned up the formula so that the A and B in the following are the former B/A and C/A),

$$1 \times (1) + A \times (2) + B \times (3) . \quad (I)$$

The requirements that f'' and f''' vanish lead to

$$1/2 + 2A + (1/2)B = 0$$

$$1/6 + (4/3)A - (1/6)B = 0$$

or

$$\begin{pmatrix} 4 & 1 \\ 8 & -1 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} -1 \\ -1 \end{pmatrix},$$

which yields $A = -1/6$, $B = -1/3$. Using these numbers, our combination (I) becomes

$$f(x_{i+1}) - (1/6)f(x_{i+2}) - (1/3)f(x_{i-1}) = (1/2)f(x_i) + f'(x_i)h + O(h^4).$$

Dividing the above formula by $6h$ yields the final result

$$f'(x_i) = (-2f(x_{i-1}) - 3f(x_i) + 6f(x_{i+1}) - f(x_{i+2})) / 6h + O(h^3).$$

Example 3. Derive the *Five-point forward difference scheme* for the *third derivative* with $O(h^2)$ error in Table 6-1 (5th formula from bottom in p. 260).
(This is a slightly more complicated case.)

First, consider the Taylor series expansion at $x = x_{i+1}, x_{i+2}, x_{i+3},$ and $x_{i+4},$

$$f(x_{i+1}) = f(x_i) + f'(x_i) h + \frac{f''(x_i) h^2}{2} + \frac{f'''(x_i) h^3}{6} + \frac{f^{(4)}(x_i) h^4}{24} + \frac{f^{(5)}(x_i) h^5}{120} + \dots \quad (1)$$

$$f(x_{i+2}) = f(x_i) + 2 f'(x_i) h + 2 f''(x_i) h^2 + \frac{4}{3} f'''(x_i) h^3 + \frac{2}{3} f^{(4)}(x_i) h^4 + \frac{8}{15} f^{(5)}(x_i) h^5 + \dots \quad (2)$$

$$f(x_{i+3}) = f(x_i) + 3 f'(x_i) h + \frac{9}{2} f''(x_i) h^2 + \frac{9}{2} f'''(x_i) h^3 + \frac{27}{8} f^{(4)}(x_i) h^4 + \frac{81}{40} f^{(5)}(x_i) h^5 + \dots \quad (3)$$

$$f(x_{i+4}) = f(x_i) + 4 f'(x_i) h + 8 f''(x_i) h^2 + \frac{32}{3} f'''(x_i) h^3 + \frac{32}{3} f^{(4)}(x_i) h^4 + \frac{128}{15} f^{(5)}(x_i) h^5 + \dots \quad (4)$$

Our goal is to combine formula (1)-(4) to eliminate all terms that involve $f', f'',$ and $f^{(4)}$ (marked in blue). This will lead to an expression of $f''' h^3$ in terms of $f(x)$ at various grid points and $f^{(5)} h^5$ plus higher order terms. Dividing that expression by h^3 yields our final formula that has $O(h^2)$ error. To proceed, we can assume that the final formula is a linear combination of (1)-(4),

$$A \times (1) + B \times (2) + C \times (3) + 1 \times (4) . \quad (I)$$

See explanation in Example 2 on why we can assign "1" as the coefficient for formula (4). We now have three unknowns and three equations

$$A + 2 B + 3 C + 4 = 0$$

$$A/2 + 2 B + (9/2) C + 8 = 0$$

$$A/24 + (2/3) B + (27/8) C + 32/3 = 0$$

or,

$$\begin{pmatrix} 1 & 2 & 3 \\ 1/2 & 2 & 9/2 \\ 1/24 & 2/3 & 27/8 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \end{pmatrix} = \begin{pmatrix} -4 \\ -8 \\ -32/3 \end{pmatrix} .$$

Solving it, we have $A = -6$, $B = 8$, and $C = -14/3$. Using these numbers, our combination (I) becomes

$$-6 f(x_{i+1}) + 8 f(x_{i+2}) - (14/3) f(x_{i+3}) + f(x_{i+4}) = - (5/3) f(x_i) - (2/3) f'''(x_i) h^3 + O(h^5) .$$

Dividing the formula by $-(2/3) h^3$ leads to the final formula in table 6-1,

$$f'''(x_i) = (-5 f(x_i) + 18 f(x_{i+1}) - 24 f(x_{i+2}) + 14 f(x_{i+3}) - 3 f(x_{i+4})) / 2h^3 + O(h^2) .$$

(Notes updated by HPH, Oct 2011)