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 $x = x_{i-1}$,

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

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

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

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

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

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

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},

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

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

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

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 $f''''(x_i)\,h^4$ 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),

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

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

$$1/2 + 2\,A + (1/2)\,B = 0$$
$$1/6 + (4/3)\,A - (1/6)\,B = 0$$

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 6 h yields the final result

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

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} ,

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

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

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

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

Our goal is to combine formula (1)-(4) to eliminate all terms that involve f', f'', and f'''' (marked in blue). This will lead to an expression of $f'''\, h^3$ in terms of $f(x)$ at various grid points and $f'''''\, h^5$ 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),

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

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,

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

(Notes updated by HPH, Oct 2011)