Question 02 a.

Use the method of undetermined coefficients to derive a difference formula for $f''(x_0)$ that uses the points $x_0, x_0 + h, x_0 + 2h$ and what is the order of the formula?

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The Taylor expansions of $f(x_0 + h)$ and $f(x_0 + 2h)$ are:

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(x_0) + \frac{h^3}{6} f'''(x_0) + \frac{h^4}{24} f^{(4)}(\xi_1) \tag{2}$$

$$f(x_0 + 2h) = f(x_0) + 2hf'(x_0) + 2h^2 f''(x_0) + \frac{4h^3}{3} f'''(x_0) + \frac{2h^4}{3} f^{(4)}(\xi_2) \tag{3}$$

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Combining (1), (2), (3):

$$
\begin{aligned}
f''(x_0) &\approx Af(x_0) + B\left(f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(x_0) + \frac{h^3}{6}f'''(x_0) + \frac{h^4}{24}f^{(4)}(\xi)\right) \\
&\quad + C\left(f(x_0) + 2hf'(x_0) + 2h^2f''(x_0) + \frac{4h^3}{3}f'''(x_0) + \frac{2h^4}{3}f^{(4)}(\xi)\right) \\
&= \left(A + B + C\right)f(x_0) + \left(B + 2C\right)hf'(x_0) + \left(\frac{B}{2} + 2C\right)h^2f''(x_0) \\
&\quad + \left(\frac{B}{6} + \frac{4C}{3}\right)h^3f'''(x_0) + \frac{B}{24}h^4f^{(4)}(\xi_1) + \frac{2C}{3}h^4f^{(4)}(\xi_2)
\end{aligned}
\tag{4}
$$

Equating the coefficients of $f(x_0), f'(x_0), f''(x_0)$ on both sides of (4) we obtain a linear system:

$$\begin{cases} 0 = \Big(A + B + C\Big) \\ 0 = \Big(B + 2C\Big)h \\ 1 = \Big(\frac{B}{2} + 2C\Big)h^2 \end{cases}$$

Solving this system we get

$$A = \frac{-1}{3h^2} \qquad B = \frac{2}{3h^2} \qquad C = \frac{-1}{3h^2} \tag{5}$$

$$\tag{6}$$

$$f''(x_0) = \frac{-f(x_0) + 2f(x_0 + h) - f(x_0 + 2h)}{3h^2} - \frac{h}{3} f'''(x_0) + \mathcal{O}(h^2) \tag{7}$$

$$f''(x_0) = \frac{-f(x_0) + 2f(x_0 + h) - f(x_0 + 2h)}{3h^2} + \mathcal{O}(h) \tag{8}$$

$$f''(x_0) \approx_0 \frac{-f(x_0) + 2f(x_0 + h) - f(x_0 + 2h)}{3h^2} \text{(First order approximation)} \tag{9}$$