Problem 2. Numerical Differentiation

Give complete details on the derivation of the five-point centered approximation to the second derivative of a function $f(x)$. Also, give complete details on using Taylor expansions to determine the leading error term.

Solution

Taylor expansions are the following:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f^{(3)}(x) + \frac{h^4}{24}f^{(4)}(x) + \Theta(h^5)$$
$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f^{(3)}(x) + \frac{h^4}{24}f^{(4)}(x) + \Theta(h^5)$$
$$f(x+2h) = f(x) + 2hf'(x) + 2h^2f''(x) + \frac{4h^3}{3}f^{(3)}(x) + \frac{2h^4}{3}f^{(4)}(x) + \Theta(h^5)$$
$$f(x-2h) = f(x) - 2hf'(x) + 2h^2f''(x) - \frac{4h^3}{3}f^{(3)}(x) + \frac{2h^4}{3}f^{(4)}(x) + \Theta(h^5)$$

We look for $\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5 \in \mathbb{R}$ for which we have:

$$f''(x) = \frac{2}{h^2}\left(\alpha_1 f(x+2h) + \alpha_2 f(x+h) + \alpha_3 f(x) + \alpha_4 f(x-h) + \alpha_5 f(x-2h)\right) + \Theta(h^3)$$

We need to solve for $\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5$ the following linear system:

$$\begin{cases} \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + \alpha_5 = 0 \\ 2\alpha_1 + \alpha_2 - \alpha_4 - \alpha_5 = 0 \\ 2\alpha_1 + \frac{1}{2}\alpha_2 + \frac{1}{2}\alpha_4 + 2\alpha_5 = \frac{1}{2} \\ \frac{4}{3}\alpha_1 + \frac{1}{6}\alpha_2 - \frac{1}{6}\alpha_4 - \frac{4}{3}\alpha_5 = 0 \\ \frac{2}{3}\alpha_1 - \frac{1}{24}\alpha_2 + \frac{1}{24}\alpha_4 + \frac{2}{3}\alpha_5 = 0 \end{cases}$$

With $\alpha_i \neq 0, \forall i \in \{1, 2, 3, 4, 5\}$.

For that, we get the following expression for f'':

$$f''(x) = \frac{-f(x+2h) + 16f(x+h) - 30f(x) + 16f(x-h) - f(x-2h)}{12h^2} + \Theta(h^3)$$

Which leaves us with an error term by h^3.