Deriving finite-difference approximation for the first and second derivative

For a well-behaved function $f(x)$, we can write the taylor expansion of $f(x+h)$ as

$$f(x+h) = f(x) + f'(x)h + \frac{f^{(2)}(x)}{2}h^2 + ... + \frac{f^{(n)}(x)}{n!}h^n + R_n(x)$$

where $R_n(x)$ is the error of truncation.

Let us consider two expansions,

$$f(x+h) = f(x) + f'(x)h + \frac{f^{(2)}(x)}{2}h^2 + R_2(x)$$

$$f(x-h) = f(x) - f'(x)h + \frac{f^{(2)}(x)}{2}h^2 + R_2(x)$$

1 First derivative

Letting $x = x_i$, we get

$$f(x_i+h) = f(x_i) + f'(x_i)h + \frac{f^{(2)}(x_i)}{2}h^2 + R_2(x_i)$$

$$f(x_i-h) = f(x_i) - f'(x_i)h + \frac{f^{(2)}(x_i)}{2}h^2 + R_2(x_i)$$

Subtracting the second from the first, we get

$$f(x_i+h) - f(x_i-h) = 2f'(x_i)h + 2R_2(x_i)$$

Dividing by $2h$ gives

$$\frac{f(x_i+h)}{2h} - \frac{f(x_i-h)}{2h} = f'(x_i) + \frac{R_2(x_i)}{h}$$

Rearranging to solve for $f'(x_i)$ gives

$$f'(x_i) = \frac{f(x_i+h) - f(x_i-h)}{2h} - \frac{R_2(x_i)}{h}$$

Assuming the error $R_2(x_i)$ is small, we can say that

$$f'(x_i) \simeq \frac{f(x_i+h) - f(x_i-h)}{2h}$$

The order of the truncation error is h^2 as R_2 contains terms h^3 and higher but the error term is $\frac{R_2(x_i)}{h}$

2 Second derivative

Letting $x = x_i$, we get

$$f(x_i+h) = f(x_i) + f'(x_i)h + \frac{f^{(2)}(x_i)}{2}h^2 + R_2(x_i)$$

$$f(x_i-h) = f(x_i) - f'(x_i)h + \frac{f^{(2)}(x_i)}{2}h^2 + R_2(x_i)$$

Adding the second to the first, we get

$$f(x_i+h) + f(x_i-h) = 2f(x_i) + f^{(2)}(x_i)h^2 + 2R_2(x_i)$$

Dividing by h^2 gives

$$\frac{f(x_i+h)}{h^2} + \frac{f(x_i-h)}{h^2} = 2\frac{f(x_i)}{h^2} + f^{(2)}(x_i) + \frac{2R_2(x_i)}{h^2}$$

Rearranging to solve for $f^{(2)}(x_i)$ gives

$$f^{(2)}(x_i) = \frac{f(x_i-h) - 2f(x_i) + f(x_i+h)}{h^2} - \frac{2R_2(x_i)}{h^2}$$

Assuming the error $R_2(x_i)$ is small, we can say that

$$f^{(2)}(x_i) \simeq \frac{f(x_i-h) - 2f(x_i) + f(x_i+h)}{h^2}$$

The order of the truncation error is h as R_2 contains terms h^3 and higher but the error term is $\frac{R_2(x_i)}{h^2}$