Substitution of derivatives by finite differences

Finite differences: Approximations of derivatives $f'(\widehat{x})$, $f''(\widehat{x})$, $\dots$ by function values $f(x_k)$ at some (finite) set of points $x_k,\ k = 1, \dots\ K$.

Taylor theorem: Let the function $f : R \to R$ be $(n+1)$ times differentiable at some open interval $I \subset R$ and let the closed interval between points $\widehat{x}$ and x lie inside I. Let $h = x - \widehat{x}$. Then

$$f(\widehat{x}+h) = f(\widehat{x}) + f'(\widehat{x})\,h + \frac{f''(\widehat{x})}{2!}\,h^2 + \cdots + \frac{f^{(n)}(\widehat{x})}{n!}\,h^n + \mathcal{O}(h^{n+1})$$

Big $\mathcal{O}$ notation $g(h) = \mathcal{O}(h^k)$ describes the limiting behavior of a function $g(h)$ as $h \to 0$: Function g is said to be $\mathcal{O}(h^k)$, if there exists a constant M such that $|g(h)| < M\,|h|^k$ at some interval $0 < |h| < h_0$.

Approximation of the first derivative:

Forward difference: Let f be twice differentiable at I, let $h > 0$. Then

$$f'(\widehat{x}) \ = \ \frac{f(\widehat{x}+h) - f(\widehat{x})}{h} + \mathcal{O}(h)$$

Backward difference: Let f be twice differentiable at I, let $h > 0$. Then

$$f'(\widehat{x}) \ = \ \frac{f(\widehat{x}) - f(\widehat{x}-h)}{h} + \mathcal{O}(h)$$

Proof follows from Taylor theorem immediatelly.

Central difference: Let f be 3 times differentiable at I, let $h > 0$. Then

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

Proof: $f(\widehat{x}+h) = f(\widehat{x}) + f'(\widehat{x})\,h + \frac{f''(\widehat{x})}{2!}\,h^2 + \mathcal{O}(h^3)$
$f(\widehat{x}-h) = f(\widehat{x}) - f'(\widehat{x})\,h + \frac{f''(\widehat{x})}{2!}\,h^2 + \mathcal{O}(h^3)$

After subtraction: $f(\widehat{x}+h) - f(\widehat{x}-h) = 2f'(\widehat{x})\,h + \mathcal{O}(h^3)$, then after division by $2h$, the desired result is obtained.

Approximation of the second derivative:

Second Central difference: Let f be 4 times differentiable at I, let $h > 0$. Then

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

Proof: $f(\widehat{x}+h) = f(\widehat{x}) + f'(\widehat{x})\,h + \frac{f''(\widehat{x})}{2!}\,h^2 + \frac{f^{(3)}(\widehat{x})}{3!}\,h^3 + \mathcal{O}(h^4)$
$f(\widehat{x}-h) = f(\widehat{x}) - f'(\widehat{x})\,h + \frac{f''(\widehat{x})}{2!}\,h^2 - \frac{f^{(3)}(\widehat{x})}{3!}\,h^3 + \mathcal{O}(h^4)$

After addition: $f(\widehat{x}+h) + f(\widehat{x}-h) = 2f(\widehat{x}) + f''(\widehat{x})\,h^2 + \mathcal{O}(h^4)$, then after division by h^2, the desired result is obtained.